Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 10:10 PM EDT

PDB ID	:	3WLW
Title	:	Molecular Architecture of the ErbB2 Extracellular Domain Homodimer
Authors	:	Hu, S.; Lou, Z.Y.; Guo, Y.J.
Deposited on	:	2013-11-15
Resolution	:	3.09 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

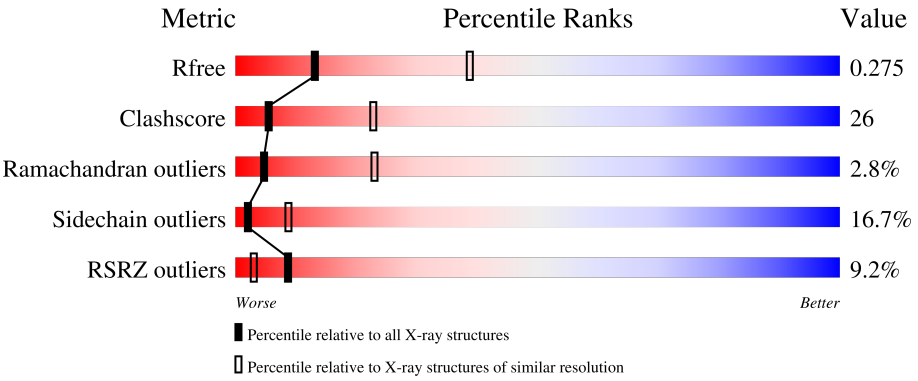
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	564	3% 60% 30% 7%
1	B	564	2% 55% 34% 9%
2	C	217	24% 43% 46% 10%
2	H	217	4% 54% 35% 9%
3	D	217	34% 43% 37% 16%

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Mol	Chain	Length	Quality of chain
3	L	217	
4	E	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	E	1	-	-	X	-
5	NAG	B	1001	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15155 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Receptor tyrosine-protein kinase erbB-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4277	2656	769	805	47			
1	B	555	Total	C	N	O	S	0	0	0
			4277	2656	769	805	47			

- Molecule 2 is a protein called Antibody H Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	217	Total	C	N	O	S	0	0	0
			1624	1021	269	327	7			
2	C	217	Total	C	N	O	S	0	0	0
			1624	1021	269	327	7			

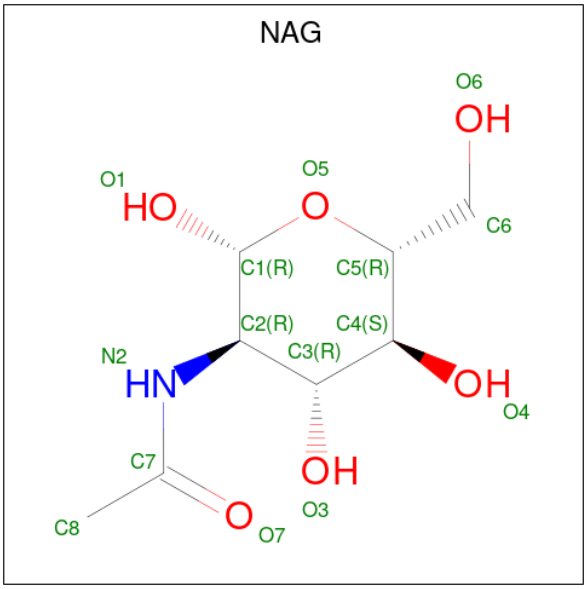
- Molecule 3 is a protein called Antibody L Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	217	Total	C	N	O	S	0	0	0
			1616	1001	269	340	6			
3	D	217	Total	C	N	O	S	0	0	0
			1616	1001	269	340	6			

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C N O 14 8 1 5	0	0

- Molecule 6 is water.

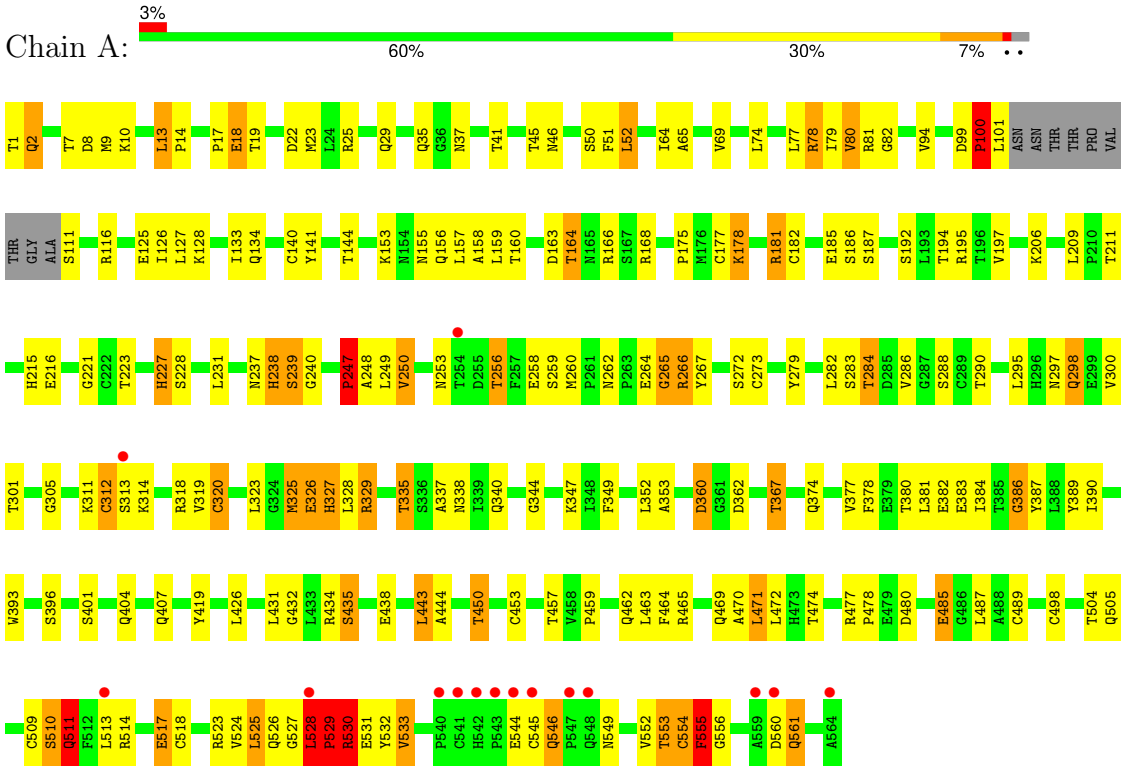
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	27	Total O 27 27	0	0
6	B	14	Total O 14 14	0	0
6	H	2	Total O 2 2	0	0
6	L	5	Total O 5 5	0	0
6	C	12	Total O 12 12	0	0
6	D	19	Total O 19 19	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

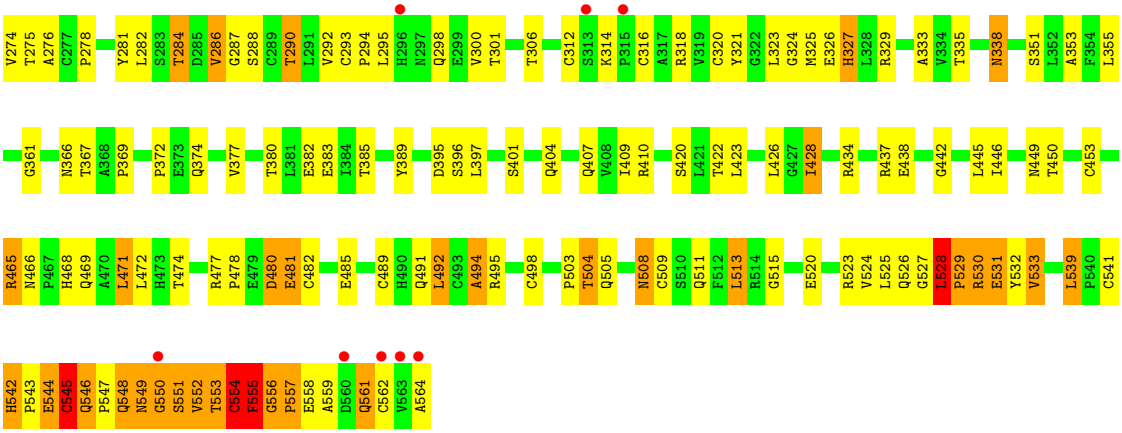
• Molecule 1: Receptor tyrosine-protein kinase erbB-2

Chain A:



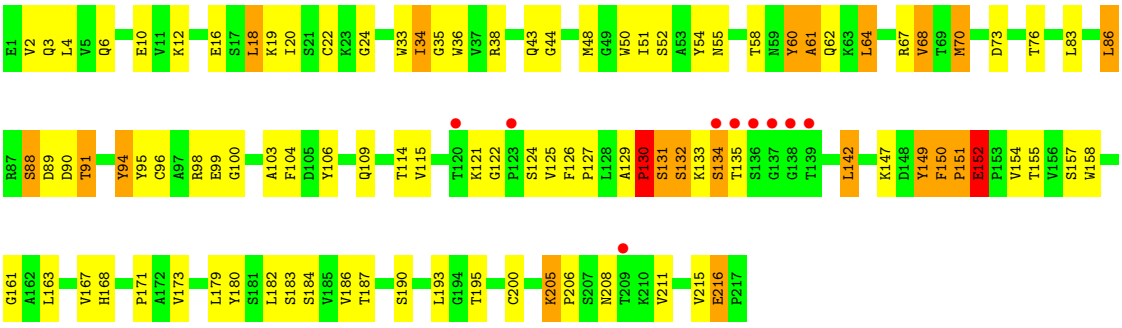
• Molecule 1: Receptor tyrosine-protein kinase erbB-2

Chain B:



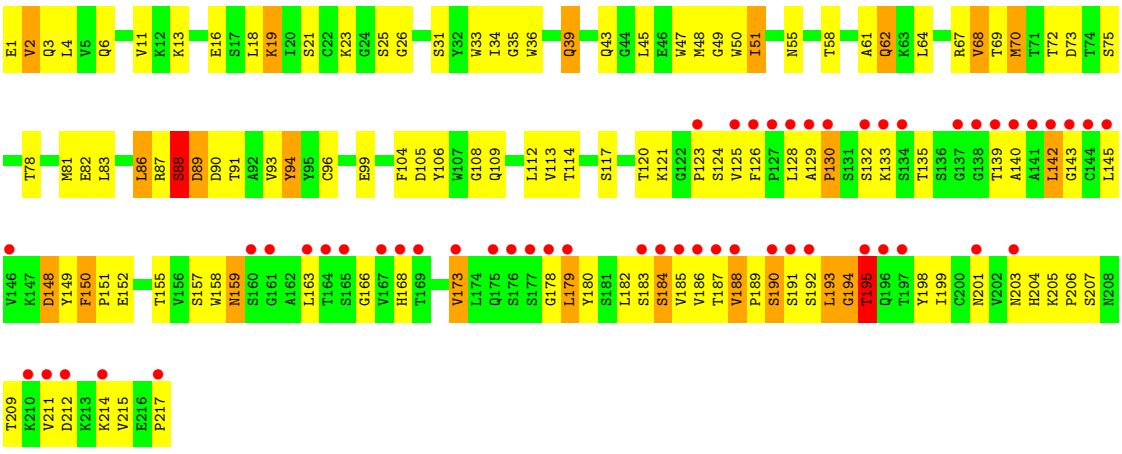
• Molecule 2: Antibody H Chain

Chain H:



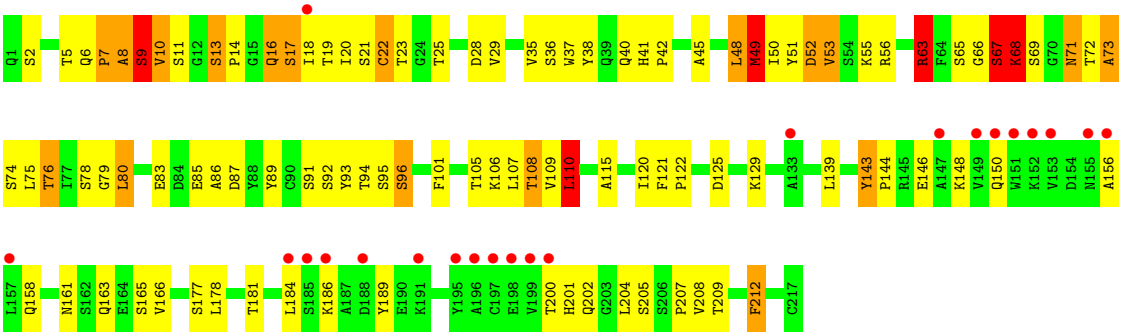
• Molecule 2: Antibody H Chain

Chain C:



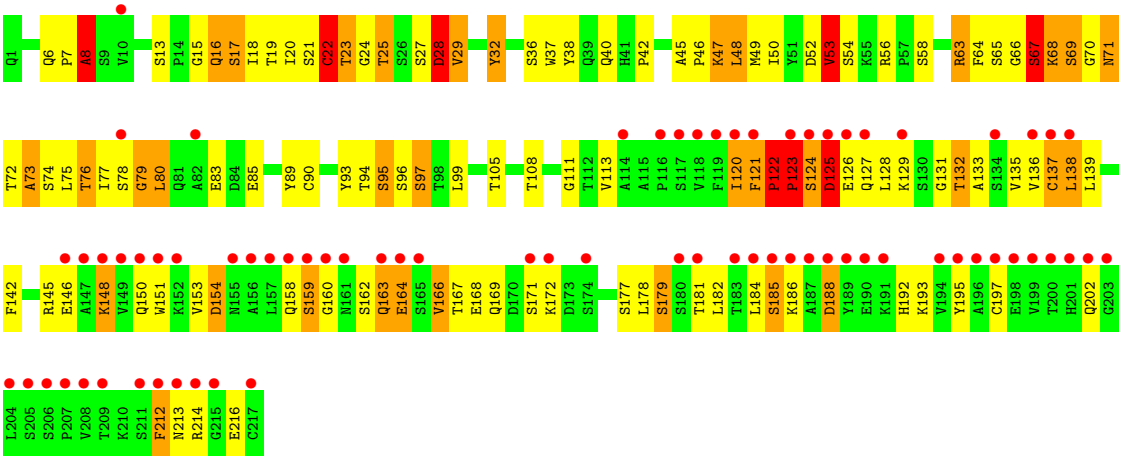
• Molecule 3: Antibody L Chain

Chain L:



• Molecule 3: Antibody L Chain

Chain D:



• Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	84.72Å 104.19Å 116.71Å 106.89° 99.65° 111.12°	Depositor
Resolution (Å)	32.26 – 3.09 48.29 – 3.09	Depositor EDS
% Data completeness (in resolution range)	97.2 (32.26-3.09) 92.3 (48.29-3.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.14 (at 3.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.232 , 0.269 0.242 , 0.275	Depositor DCC
R_{free} test set	3059 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	62.5	Xtriage
Anisotropy	0.581	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 68.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	15155	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.58	3/4374 (0.1%)	0.91	24/5950 (0.4%)
1	B	0.59	2/4374 (0.0%)	0.88	13/5950 (0.2%)
2	C	0.46	0/1664	0.78	5/2268 (0.2%)
2	H	0.50	1/1664 (0.1%)	0.91	10/2268 (0.4%)
3	D	0.60	0/1649	1.08	18/2241 (0.8%)
3	L	0.55	0/1649	1.02	12/2241 (0.5%)
All	All	0.56	6/15374 (0.0%)	0.92	82/20918 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	1
2	C	0	2
2	H	0	1
3	D	0	6
3	L	0	4
All	All	0	17

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	539	LEU	C-N	10.37	1.53	1.34
1	A	265	GLY	C-N	8.59	1.53	1.34
1	A	247	PRO	C-N	6.51	1.49	1.34
1	B	557	PRO	N-CD	5.63	1.55	1.47
1	A	529	PRO	N-CD	5.28	1.55	1.47
2	H	130	PRO	N-CD	5.18	1.55	1.47

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	326	GLU	CB-CA-C	-11.98	86.43	110.40
1	B	269	PHE	CB-CA-C	11.84	134.09	110.40
2	H	62	GLN	N-CA-CB	-10.85	91.07	110.60
1	A	510	SER	CB-CA-C	-10.46	90.22	110.10
3	L	48	LEU	N-CA-CB	-10.30	89.81	110.40
1	A	546	GLN	N-CA-CB	-10.10	92.42	110.60
3	L	53	VAL	N-CA-CB	9.46	132.31	111.50
3	D	67	SER	CB-CA-C	-9.11	92.79	110.10
3	D	7	PRO	N-CA-C	8.94	135.34	112.10
1	A	240	GLY	N-CA-C	-8.92	90.81	113.10
2	H	132	SER	N-CA-C	-8.29	88.63	111.00
3	D	7	PRO	CB-CA-C	-8.23	91.42	112.00
3	L	9	SER	CB-CA-C	-8.12	94.67	110.10
2	H	60	TYR	CB-CA-C	-8.08	94.23	110.40
3	D	125	ASP	CB-CA-C	-7.81	94.78	110.40
3	D	79	GLY	N-CA-C	-7.76	93.70	113.10
1	B	494	ALA	CB-CA-C	-7.75	98.48	110.10
2	H	132	SER	N-CA-CB	7.68	122.03	110.50
3	D	53	VAL	N-CA-CB	7.64	128.32	111.50
1	A	325	MET	CB-CA-C	7.53	125.47	110.40
1	A	197	VAL	N-CA-CB	-7.46	95.09	111.50
2	H	61	ALA	CB-CA-C	-7.46	98.92	110.10
3	L	17	SER	N-CA-C	-7.35	91.14	111.00
1	A	546	GLN	N-CA-C	7.34	130.83	111.00
3	L	110	LEU	CA-CB-CG	7.13	131.70	115.30
3	D	23	THR	N-CA-C	-7.13	91.75	111.00
1	A	511	GLN	N-CA-CB	7.04	123.27	110.60
1	A	545	CYS	N-CA-CB	-7.03	97.94	110.60
1	A	387	TYR	N-CA-CB	-6.94	98.10	110.60
2	H	90	ASP	N-CA-C	-6.80	92.63	111.00
1	B	100	PRO	N-CA-C	6.75	129.65	112.10
1	B	161	LEU	CA-CB-CG	6.73	130.77	115.30
2	C	62	GLN	CB-CA-C	-6.61	97.19	110.40
1	B	428	ILE	CB-CA-C	-6.56	98.48	111.60
2	C	195	THR	N-CA-CB	-6.54	97.87	110.30
2	C	89	ASP	N-CA-C	-6.52	93.39	111.00
1	A	313	SER	CB-CA-C	-6.40	97.95	110.10
1	B	530	ARG	N-CA-C	6.38	128.22	111.00
1	B	7	THR	CB-CA-C	-6.37	94.41	111.60
2	H	61	ALA	N-CA-CB	-6.27	101.32	110.10
3	L	9	SER	CA-C-N	-6.27	103.40	117.20
3	D	28	ASP	CB-CA-C	-6.17	98.07	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	177	CYS	CB-CA-C	6.08	122.56	110.40
3	L	49	MET	N-CA-C	-6.08	94.58	111.00
3	L	53	VAL	N-CA-C	-6.01	94.78	111.00
3	D	28	ASP	N-CA-C	5.99	127.18	111.00
2	C	88	SER	N-CA-C	-5.94	94.95	111.00
3	L	67	SER	CB-CA-C	-5.93	98.84	110.10
3	D	121	PHE	C-N-CD	-5.91	107.60	120.60
3	L	68	LYS	N-CA-C	5.78	126.61	111.00
3	D	69	SER	CB-CA-C	5.76	121.04	110.10
3	D	122	PRO	C-N-CD	5.75	140.48	128.40
3	D	123	PRO	CA-N-CD	-5.72	103.49	111.50
2	H	129	ALA	C-N-CD	5.70	140.37	128.40
1	A	511	GLN	N-CA-C	-5.69	95.63	111.00
2	H	94	TYR	N-CA-C	5.68	126.33	111.00
1	A	100	PRO	N-CA-C	5.63	126.73	112.10
3	D	8	ALA	CB-CA-C	-5.56	101.76	110.10
1	A	314	LYS	N-CA-C	-5.51	96.13	111.00
3	L	52	ASP	CB-CA-C	5.49	121.38	110.40
1	A	386	GLY	N-CA-C	-5.45	99.47	113.10
1	B	531	GLU	N-CA-C	5.38	125.53	111.00
2	C	94	TYR	N-CA-C	5.35	125.45	111.00
1	A	431	LEU	CB-CA-C	-5.35	100.03	110.20
3	D	22	CYS	N-CA-C	5.31	125.34	111.00
1	B	271	ALA	N-CA-CB	5.23	117.43	110.10
1	B	29	GLN	N-CA-C	5.22	125.09	111.00
1	A	100	PRO	CB-CA-C	-5.20	99.01	112.00
1	A	528	LEU	C-N-CD	5.20	139.31	128.40
3	D	160	GLY	N-CA-C	-5.19	100.13	113.10
1	B	556	GLY	C-N-CD	5.19	139.29	128.40
2	H	142	LEU	CA-CB-CG	5.18	127.21	115.30
1	A	78	ARG	NE-CZ-NH2	-5.14	117.73	120.30
3	D	29	VAL	N-CA-C	-5.13	97.16	111.00
1	A	432	GLY	N-CA-C	5.11	125.87	113.10
1	A	195	ARG	CB-CA-C	-5.10	100.21	110.40
3	D	32	TYR	N-CA-C	5.08	124.72	111.00
1	B	269	PHE	N-CA-C	-5.06	97.34	111.00
1	A	101	LEU	N-CA-CB	5.05	120.49	110.40
1	A	544	GLU	CB-CA-C	-5.03	100.35	110.40
1	B	539	LEU	O-C-N	5.02	130.64	121.10
3	L	143	TYR	N-CA-C	-5.01	97.47	111.00

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	111	SER	Peptide
1	A	247	PRO	Mainchain
1	A	77	LEU	Peptide
1	B	529	PRO	Peptide
2	C	190	SER	Peptide
2	C	88	SER	Peptide
3	D	121	PHE	Mainchain
3	D	159	SER	Peptide
3	D	22	CYS	Peptide
3	D	63	ARG	Peptide
3	D	67	SER	Peptide
3	D	8	ALA	Peptide
2	H	152	GLU	Peptide
3	L	16	GLN	Peptide
3	L	22	CYS	Peptide
3	L	63	ARG	Peptide
3	L	67	SER	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4277	0	4106	142	0
1	B	4277	0	4108	216	3
2	C	1624	0	1567	110	2
2	H	1624	0	1567	81	1
3	D	1616	0	1548	148	0
3	L	1616	0	1548	89	0
4	E	28	0	25	8	0
5	B	14	0	13	10	0
6	A	27	0	0	4	0
6	B	14	0	0	1	0
6	C	12	0	0	7	0
6	D	19	0	0	4	0
6	H	2	0	0	0	0
6	L	5	0	0	1	0
All	All	15155	0	14482	766	3

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (766) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:546:GLN:CG	1:B:548:GLN:HG3	1.37	1.53
3:D:123:PRO:HB2	3:D:127:GLN:CD	1.29	1.48
1:A:237:ASN:HD21	4:E:1:NAG:C1	1.21	1.47
3:D:123:PRO:CB	3:D:127:GLN:NE2	1.79	1.44
1:B:250:VAL:CB	1:B:260:MET:O	1.69	1.39
1:B:546:GLN:HG2	1:B:548:GLN:CG	1.52	1.36
2:H:131:SER:OG	2:H:133:LYS:HB3	1.23	1.33
3:D:123:PRO:HB2	3:D:127:GLN:NE2	1.01	1.32
2:H:131:SER:OG	2:H:133:LYS:CB	1.77	1.31
1:A:553:THR:HG22	6:A:1114:HOH:O	1.36	1.24
1:B:250:VAL:HG12	1:B:261:PRO:CA	1.67	1.23
1:B:250:VAL:HB	1:B:260:MET:O	1.12	1.23
1:A:238:HIS:HB2	1:A:273:CYS:SG	1.79	1.22
2:H:131:SER:OG	2:H:133:LYS:CA	1.88	1.21
2:H:131:SER:OG	2:H:133:LYS:N	1.73	1.21
3:D:23:THR:CG2	3:D:72:THR:HG22	1.69	1.20
1:B:549:ASN:O	1:B:550:GLY:O	1.60	1.20
3:D:22:CYS:CB	3:D:73:ALA:HB1	1.71	1.19
1:B:250:VAL:CG1	1:B:261:PRO:HA	1.76	1.16
2:C:128:LEU:HD22	3:D:122:PRO:O	1.43	1.15
3:L:94:THR:HG22	3:L:96:SER:H	1.12	1.15
3:D:22:CYS:HB2	3:D:73:ALA:CB	1.74	1.15
1:A:553:THR:CG2	6:A:1114:HOH:O	1.90	1.13
1:A:528:LEU:O	1:A:530:ARG:N	1.83	1.11
1:B:237:ASN:CG	5:B:1001:NAG:C1	2.19	1.08
1:B:546:GLN:O	1:B:548:GLN:N	1.86	1.08
1:B:250:VAL:CG1	1:B:260:MET:O	2.02	1.08
1:A:326:GLU:O	1:A:327:HIS:HB3	1.54	1.07
1:B:545:CYS:SG	1:B:562:CYS:SG	1.31	1.07
3:D:23:THR:HG22	3:D:72:THR:HG22	1.35	1.06
1:A:528:LEU:HB2	1:A:529:PRO:HD3	1.37	1.05
1:B:247:PRO:HB2	1:B:265:GLY:HA2	1.32	1.04
2:C:128:LEU:CD2	3:D:122:PRO:O	2.05	1.04
2:C:130:PRO:HG2	2:C:193:LEU:HD11	1.38	1.04
3:D:131:GLY:HA2	3:D:186:LYS:HB2	1.40	1.04
1:B:542:HIS:CE1	1:B:543:PRO:HD2	1.92	1.04
1:B:546:GLN:CG	1:B:548:GLN:CG	2.23	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:130:PRO:HG3	2:C:142:LEU:HB3	1.38	1.02
1:A:528:LEU:C	1:A:530:ARG:H	1.63	1.01
3:D:24:GLY:O	3:D:71:ASN:HB3	1.63	0.99
1:B:553:THR:HG22	1:B:554:CYS:H	1.24	0.99
3:D:67:SER:O	3:D:68:LYS:HB2	1.58	0.98
1:B:545:CYS:O	1:B:546:GLN:HB2	1.61	0.98
3:L:9:SER:C	3:L:11:SER:H	1.66	0.98
2:C:189:PRO:HB3	2:C:191:SER:HB3	1.42	0.98
1:B:237:ASN:ND2	5:B:1001:NAG:O5	1.94	0.97
3:L:9:SER:O	3:L:11:SER:N	1.96	0.97
3:D:123:PRO:CB	3:D:127:GLN:CD	2.19	0.96
1:A:384:ILE:HG22	1:A:386:GLY:O	1.65	0.95
3:D:94:THR:HG22	3:D:96:SER:H	1.28	0.95
1:B:546:GLN:HE21	1:B:548:GLN:CB	1.79	0.95
1:B:541:CYS:O	1:B:542:HIS:O	1.84	0.95
1:B:553:THR:HG22	1:B:554:CYS:N	1.82	0.95
3:D:23:THR:CG2	3:D:72:THR:CG2	2.46	0.94
3:D:123:PRO:CA	3:D:127:GLN:NE2	2.31	0.94
1:A:554:CYS:SG	1:A:555:PHE:N	2.35	0.94
2:H:131:SER:HG	2:H:133:LYS:HB3	1.12	0.94
1:B:546:GLN:C	1:B:548:GLN:H	1.69	0.93
1:A:528:LEU:HB2	1:A:529:PRO:CD	1.98	0.93
3:D:16:GLN:HA	3:D:17:SER:HB3	1.51	0.93
3:L:72:THR:HA	3:L:73:ALA:HB3	1.48	0.93
1:B:250:VAL:HG12	1:B:261:PRO:HA	0.94	0.92
3:D:23:THR:CB	3:D:72:THR:HG22	1.98	0.92
1:A:237:ASN:HD21	4:E:1:NAG:C2	1.82	0.91
3:D:69:SER:O	3:D:72:THR:O	1.87	0.91
3:L:9:SER:OG	3:L:10:VAL:N	1.98	0.91
1:B:237:ASN:HD21	5:B:1001:NAG:C1	1.56	0.91
3:L:35:VAL:O	3:L:52:ASP:O	1.91	0.89
1:B:545:CYS:CB	1:B:562:CYS:SG	2.61	0.88
3:D:72:THR:HA	3:D:73:ALA:HB3	1.56	0.87
1:B:545:CYS:O	1:B:546:GLN:CB	2.22	0.87
2:H:131:SER:HG	2:H:133:LYS:CB	1.73	0.87
2:C:51:ILE:HG12	2:C:58:THR:HG22	1.54	0.86
1:B:327:HIS:O	1:B:327:HIS:CD2	2.28	0.86
3:D:16:GLN:CA	3:D:17:SER:HB3	2.05	0.86
1:A:510:SER:O	1:A:511:GLN:OE1	1.94	0.86
2:C:203:ASN:HD21	2:C:205:LYS:HG3	1.40	0.86
1:B:546:GLN:NE2	1:B:548:GLN:HB2	1.89	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:528:LEU:HB2	1:B:529:PRO:HD3	1.56	0.85
3:L:13:SER:HA	3:L:110:LEU:HB2	1.56	0.85
4:E:1:NAG:O3	4:E:2:NAG:O5	1.93	0.85
1:A:238:HIS:HB2	1:A:273:CYS:CB	2.06	0.85
3:L:72:THR:HA	3:L:73:ALA:CB	2.07	0.84
1:B:250:VAL:HA	1:B:262:ASN:H	1.42	0.83
1:B:553:THR:O	1:B:554:CYS:O	1.95	0.83
1:A:532:TYR:HB3	1:A:554:CYS:SG	2.17	0.83
3:D:23:THR:HB	3:D:72:THR:CG2	2.08	0.83
2:C:142:LEU:HD22	2:C:193:LEU:HD12	1.60	0.83
2:H:131:SER:CB	2:H:133:LYS:HB3	2.09	0.83
1:B:546:GLN:NE2	1:B:548:GLN:CB	2.41	0.82
1:B:83:THR:HG22	1:B:84:GLN:HG3	1.61	0.82
1:B:546:GLN:HG3	1:B:548:GLN:HG3	1.58	0.82
3:D:72:THR:HA	3:D:73:ALA:CB	2.10	0.82
3:L:29:VAL:HG21	3:L:73:ALA:HB2	1.59	0.82
1:A:144:THR:HG21	1:A:182:CYS:H	1.44	0.81
1:B:546:GLN:HE21	1:B:548:GLN:CD	1.83	0.81
3:D:123:PRO:HB2	3:D:127:GLN:HE21	1.41	0.81
1:B:250:VAL:HG12	1:B:260:MET:O	1.76	0.81
2:C:139:THR:O	6:C:308:HOH:O	1.98	0.81
1:B:272:SER:HB3	5:B:1001:NAG:O7	1.81	0.81
3:D:123:PRO:C	3:D:127:GLN:HE21	1.84	0.81
1:A:524:VAL:HG11	1:A:533:VAL:HG22	1.61	0.81
1:B:553:THR:CG2	1:B:554:CYS:H	1.82	0.81
2:H:131:SER:CB	2:H:133:LYS:H	1.94	0.81
2:H:60:TYR:HE1	2:H:70:MET:HG3	1.45	0.80
1:B:140:CYS:HA	1:B:166:ARG:HH21	1.45	0.80
3:L:40:GLN:O	3:L:86:ALA:HB1	1.81	0.80
1:B:523:ARG:HG2	1:B:527:GLY:HA3	1.62	0.80
2:C:51:ILE:HG13	2:C:70:MET:HB2	1.62	0.80
3:D:23:THR:HB	3:D:72:THR:HG22	1.62	0.79
2:C:142:LEU:CD2	2:C:193:LEU:HD12	2.12	0.79
1:B:428:ILE:O	1:B:428:ILE:HG13	1.81	0.79
3:D:120:ILE:HD12	3:D:212:PHE:HB3	1.62	0.79
1:A:253:ASN:ND2	1:A:256:THR:OG1	2.13	0.79
3:L:23:THR:HB	3:L:72:THR:OG1	1.82	0.79
1:B:545:CYS:SG	1:B:562:CYS:CB	2.72	0.78
1:B:546:GLN:HE21	1:B:548:GLN:CG	1.96	0.78
2:C:128:LEU:HD23	3:D:123:PRO:HA	1.64	0.78
1:B:250:VAL:HB	1:B:260:MET:C	2.05	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:91:THR:HG23	2:H:114:THR:HA	1.68	0.76
1:A:362:ASP:HB3	1:A:367:THR:HG23	1.66	0.76
3:L:20:ILE:HD12	3:L:20:ILE:H	1.50	0.76
2:C:193:LEU:HA	2:C:198:TYR:HE2	1.50	0.76
2:C:133:LYS:HZ1	3:D:212:PHE:HB2	1.51	0.76
3:D:123:PRO:CB	3:D:127:GLN:HE22	1.94	0.75
1:A:18:GLU:N	1:A:18:GLU:OE1	2.18	0.75
1:A:238:HIS:CB	1:A:273:CYS:SG	2.69	0.75
2:H:190:SER:HA	2:H:193:LEU:HD13	1.67	0.75
1:B:546:GLN:HG3	1:B:548:GLN:HE21	1.49	0.75
3:L:20:ILE:HD12	3:L:20:ILE:N	2.02	0.75
1:B:237:ASN:HD21	5:B:1001:NAG:H61	1.52	0.75
3:D:123:PRO:C	3:D:127:GLN:NE2	2.40	0.75
2:C:142:LEU:HD22	2:C:193:LEU:CD1	2.16	0.75
1:B:250:VAL:CA	1:B:260:MET:O	2.34	0.74
2:H:48:MET:HG2	2:H:64:LEU:HD21	1.68	0.74
1:B:541:CYS:C	1:B:542:HIS:O	2.23	0.74
1:A:250:VAL:HG21	1:A:259:SER:HB3	1.70	0.73
3:L:94:THR:HG22	3:L:96:SER:N	1.97	0.73
2:C:158:TRP:HZ3	2:C:198:TYR:HB3	1.50	0.73
1:B:81:ARG:HG2	1:B:127:LEU:HD12	1.70	0.73
1:A:326:GLU:O	1:A:327:HIS:CB	2.34	0.73
2:H:89:ASP:CG	2:H:89:ASP:O	2.24	0.73
1:B:438:GLU:OE2	1:B:465:ARG:NH1	2.22	0.73
1:B:542:HIS:NE2	1:B:543:PRO:HD2	2.03	0.72
1:B:546:GLN:HG3	1:B:548:GLN:NE2	2.04	0.72
1:A:528:LEU:HD23	1:A:528:LEU:N	2.05	0.72
1:A:256:THR:HB	1:A:258:GLU:HG3	1.71	0.71
1:B:530:ARG:O	1:B:530:ARG:HG3	1.88	0.71
1:A:453:CYS:SG	1:A:477:ARG:NH1	2.63	0.71
3:L:83:GLU:HA	3:L:85:GLU:HG3	1.73	0.71
2:C:194:GLY:HA3	2:C:217:PRO:HG2	1.72	0.71
1:B:22:ASP:OD1	1:B:25:ARG:NH1	2.23	0.71
3:L:14:PRO:HD3	3:L:110:LEU:H	1.56	0.71
3:D:123:PRO:O	3:D:124:SER:OG	2.07	0.71
1:A:140:CYS:HA	1:A:166:ARG:HH21	1.54	0.71
3:L:41:HIS:HB3	3:L:42:PRO:HD2	1.71	0.71
3:L:16:GLN:HB2	3:L:17:SER:OG	1.91	0.71
1:B:237:ASN:HD21	5:B:1001:NAG:C6	2.04	0.70
1:B:546:GLN:HG2	1:B:548:GLN:CB	2.21	0.70
3:D:50:ILE:HG21	3:D:56:ARG:HG2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:PRO:O	1:A:530:ARG:O	2.10	0.69
3:L:22:CYS:HB3	3:L:23:THR:HA	1.74	0.69
2:H:16:GLU:O	2:H:86:LEU:HB2	1.92	0.69
3:L:5:THR:O	3:L:22:CYS:O	2.11	0.69
1:A:279:TYR:OH	1:A:438:GLU:OE2	2.11	0.69
1:B:524:VAL:HG11	1:B:533:VAL:HG22	1.76	0.68
1:A:347:LYS:HE2	1:A:349:PHE:CZ	2.28	0.68
1:B:237:ASN:OD1	5:B:1001:NAG:C1	2.42	0.68
3:D:133:ALA:N	3:D:184:LEU:O	2.26	0.68
1:B:237:ASN:HD21	5:B:1001:NAG:C5	2.05	0.68
2:H:131:SER:O	2:H:135:THR:HG23	1.94	0.68
3:L:5:THR:O	3:L:22:CYS:C	2.33	0.68
3:L:67:SER:O	3:L:68:LYS:HB2	1.92	0.68
1:B:33:VAL:HG13	1:B:57:GLU:HB2	1.76	0.68
1:B:541:CYS:O	1:B:542:HIS:C	2.32	0.68
2:H:51:ILE:HG12	2:H:58:THR:HG22	1.75	0.67
1:B:542:HIS:CG	1:B:543:PRO:CD	2.77	0.67
3:D:124:SER:C	3:D:126:GLU:H	1.98	0.67
1:A:249:LEU:HD11	1:A:267:TYR:CZ	2.28	0.67
2:C:151:PRO:HD2	2:C:206:PRO:HB3	1.77	0.67
3:D:111:GLY:O	6:D:314:HOH:O	2.12	0.67
1:B:494:ALA:HB3	1:B:508:ASN:HB3	1.76	0.67
2:H:64:LEU:HB3	2:H:68:VAL:HG22	1.76	0.66
1:B:263:PRO:O	1:B:264:GLU:HG2	1.96	0.66
2:H:150:PHE:HD2	2:H:179:LEU:HD23	1.60	0.66
3:D:52:ASP:O	3:D:53:VAL:HG22	1.96	0.66
3:D:18:ILE:HG22	3:D:19:THR:H	1.59	0.66
3:L:143:TYR:O	3:L:201:HIS:NE2	2.29	0.66
3:D:67:SER:O	3:D:68:LYS:CB	2.41	0.66
1:B:374:GLN:O	1:B:377:VAL:HG13	1.94	0.66
2:C:91:THR:HG23	2:C:114:THR:HA	1.77	0.66
3:D:150:GLN:O	6:D:307:HOH:O	2.13	0.66
1:B:247:PRO:CB	1:B:265:GLY:HA2	2.19	0.66
3:D:8:ALA:HA	3:D:105:THR:HA	1.78	0.66
3:D:94:THR:HG22	3:D:96:SER:N	2.07	0.65
2:C:183:SER:OG	2:C:184:SER:N	2.29	0.65
3:D:16:GLN:HA	3:D:17:SER:CB	2.26	0.65
1:A:407:GLN:HA	1:A:435:SER:O	1.97	0.65
3:D:23:THR:HG21	3:D:72:THR:CG2	2.25	0.65
1:B:284:THR:HG22	1:B:287:GLY:H	1.62	0.65
1:A:266:ARG:HG2	1:A:266:ARG:HH11	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:130:PRO:O	2:H:131:SER:HB3	1.96	0.65
3:D:139:LEU:HD22	3:D:178:LEU:HB3	1.79	0.65
1:A:22:ASP:OD1	1:A:25:ARG:NH1	2.29	0.65
1:B:546:GLN:NE2	1:B:548:GLN:CD	2.50	0.65
2:C:139:THR:HA	2:C:190:SER:H	1.60	0.65
1:B:284:THR:HG22	1:B:288:SER:H	1.62	0.64
1:B:144:THR:HG21	1:B:182:CYS:H	1.62	0.64
2:H:125:VAL:HG21	2:H:211:VAL:HG11	1.79	0.64
3:D:139:LEU:HB3	3:D:142:PHE:CE2	2.33	0.64
1:A:51:PHE:CE1	1:A:52:LEU:HD13	2.32	0.64
1:A:404:GLN:OE1	1:A:434:ARG:NH1	2.30	0.64
3:L:8:ALA:HA	3:L:106:LYS:H	1.61	0.64
1:A:528:LEU:C	1:A:530:ARG:N	2.33	0.64
1:B:132:LEU:HD13	1:B:161:LEU:HD23	1.80	0.64
1:B:250:VAL:CG1	1:B:260:MET:C	2.64	0.64
1:B:542:HIS:HB2	1:B:557:PRO:O	1.97	0.64
3:D:25:THR:N	3:D:28:ASP:OD2	2.28	0.64
1:B:325:MET:O	1:B:329:ARG:HB3	1.98	0.63
3:D:23:THR:HB	3:D:72:THR:HG23	1.80	0.63
3:D:139:LEU:HB3	3:D:142:PHE:HE2	1.61	0.63
1:B:324:GLY:HA2	1:B:329:ARG:HA	1.81	0.63
1:B:542:HIS:CD2	1:B:543:PRO:HD2	2.32	0.63
2:C:51:ILE:HG21	2:C:72:THR:HG23	1.81	0.63
3:D:17:SER:HB3	3:D:78:SER:O	1.98	0.63
1:A:459:PRO:HB2	1:A:462:GLN:HG3	1.81	0.63
3:D:23:THR:CB	3:D:72:THR:CG2	2.67	0.63
1:B:237:ASN:ND2	5:B:1001:NAG:H61	2.14	0.62
1:B:546:GLN:NE2	1:B:548:GLN:CG	2.61	0.62
1:A:265:GLY:O	1:A:266:ARG:HD3	1.99	0.62
3:D:22:CYS:HB2	3:D:73:ALA:HB1	0.81	0.62
3:D:132:THR:HA	3:D:185:SER:HA	1.82	0.62
2:C:135:THR:HA	6:C:308:HOH:O	1.98	0.62
3:D:24:GLY:O	3:D:71:ASN:CB	2.44	0.62
1:B:327:HIS:O	1:B:327:HIS:CG	2.48	0.62
1:B:383:GLU:OE1	1:B:410:ARG:NE	2.27	0.62
1:A:238:HIS:HB2	1:A:273:CYS:HB2	1.80	0.62
1:B:250:VAL:HA	1:B:262:ASN:N	2.13	0.62
1:B:335:THR:N	1:B:338:ASN:OD1	2.29	0.62
2:H:6:GLN:H	2:H:109:GLN:HE22	1.47	0.62
1:B:478:PRO:HB2	1:B:481:GLU:HB2	1.81	0.62
3:D:182:LEU:HG	3:D:184:LEU:HG	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:7:PRO:HG2	3:L:105:THR:HG21	1.82	0.62
3:L:78:SER:OG	3:L:79:GLY:N	2.29	0.62
3:D:16:GLN:CB	3:D:17:SER:HB3	2.30	0.62
1:A:335:THR:HG23	1:A:337:ALA:H	1.65	0.61
1:A:175:PRO:O	3:D:32:TYR:OH	2.13	0.61
1:B:7:THR:O	1:B:39:GLU:OE1	2.18	0.61
1:B:144:THR:CG2	1:B:182:CYS:H	2.13	0.61
2:C:194:GLY:CA	2:C:217:PRO:HD2	2.30	0.61
2:H:51:ILE:HD11	2:H:70:MET:C	2.22	0.61
3:D:8:ALA:H	3:D:105:THR:HG22	1.65	0.61
1:A:141:TYR:OH	1:A:185:GLU:HG2	2.00	0.61
3:D:123:PRO:HB2	3:D:127:GLN:CG	2.25	0.61
3:L:143:TYR:O	3:L:201:HIS:CE1	2.54	0.60
2:C:189:PRO:HB2	2:C:192:SER:H	1.66	0.60
1:A:94:VAL:HG22	1:A:133:ILE:HG23	1.83	0.60
1:A:298:GLN:HG2	1:A:312:CYS:SG	2.41	0.60
3:L:71:ASN:OD1	3:L:71:ASN:N	2.32	0.60
2:H:171:PRO:HG2	3:L:166:VAL:H	1.66	0.60
3:D:108:THR:OG1	3:D:169:GLN:NE2	2.33	0.60
1:B:546:GLN:HG2	1:B:548:GLN:HG3	0.64	0.60
1:B:542:HIS:ND1	1:B:543:PRO:HD2	2.16	0.60
1:B:552:VAL:O	1:B:552:VAL:HG13	2.01	0.60
2:C:188:VAL:HG11	2:C:198:TYR:HE1	1.66	0.60
3:D:15:GLY:O	3:D:16:GLN:HB3	2.02	0.60
1:B:284:THR:HG23	1:B:286:VAL:HG13	1.83	0.59
1:B:542:HIS:CD2	1:B:543:PRO:CD	2.86	0.59
3:D:19:THR:HG22	3:D:76:THR:HB	1.85	0.59
3:D:135:VAL:HB	3:D:182:LEU:HD23	1.85	0.59
1:B:300:VAL:HG12	1:B:301:THR:H	1.67	0.59
2:H:60:TYR:CE1	2:H:70:MET:HG3	2.32	0.59
3:L:9:SER:C	3:L:11:SER:N	2.33	0.58
1:A:144:THR:CG2	1:A:182:CYS:H	2.13	0.58
2:C:193:LEU:HA	2:C:198:TYR:CE2	2.35	0.58
3:L:19:THR:HG22	3:L:76:THR:HB	1.83	0.58
3:D:42:PRO:HG3	3:D:168:GLU:HG3	1.84	0.58
1:B:7:THR:OG1	1:B:39:GLU:OE1	2.19	0.58
2:C:18:LEU:HB2	2:C:86:LEU:HD21	1.86	0.58
1:A:523:ARG:HB2	1:A:531:GLU:HB2	1.85	0.58
1:B:51:PHE:CE1	1:B:52:LEU:HD13	2.38	0.58
1:B:209:LEU:HB3	1:B:211:THR:HG22	1.85	0.58
1:B:250:VAL:HG12	1:B:260:MET:C	2.23	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:36:TRP:CE2	2:C:81:MET:HB2	2.39	0.58
3:D:128:LEU:HA	3:D:132:THR:O	2.03	0.58
1:A:141:TYR:O	1:A:144:THR:HG22	2.04	0.57
1:A:237:ASN:ND2	4:E:1:NAG:C7	2.67	0.57
1:B:274:VAL:HG12	1:B:276:ALA:H	1.69	0.57
3:L:16:GLN:HA	3:L:78:SER:O	2.05	0.57
3:L:35:VAL:HB	3:L:53:VAL:HG12	1.86	0.57
2:H:89:ASP:O	2:H:89:ASP:OD2	2.23	0.57
1:A:238:HIS:HA	1:A:273:CYS:HB2	1.84	0.57
1:B:58:VAL:HG11	1:B:62:VAL:HG22	1.86	0.57
3:D:17:SER:CB	3:D:78:SER:O	2.52	0.57
2:C:125:VAL:HG11	2:C:211:VAL:HG11	1.87	0.57
2:C:193:LEU:O	2:C:195:THR:CB	2.53	0.57
1:B:9:MET:O	1:B:12:ARG:HB2	2.05	0.56
2:H:149:TYR:CE1	2:H:180:TYR:HB2	2.40	0.56
3:D:72:THR:CA	3:D:73:ALA:HB3	2.32	0.56
1:A:352:LEU:HD12	1:A:384:ILE:HD11	1.87	0.56
3:D:123:PRO:HD2	3:D:124:SER:H	1.70	0.56
1:A:284:THR:HG22	1:A:288:SER:H	1.70	0.56
1:B:248:ALA:O	1:B:262:ASN:HB3	2.06	0.56
2:H:51:ILE:HG22	2:H:52:SER:N	2.20	0.56
3:D:145:ARG:NH2	3:D:166:VAL:HG11	2.20	0.56
1:B:194:THR:OG1	1:B:204:ARG:NH1	2.36	0.56
1:B:544:GLU:O	1:B:545:CYS:HB2	2.05	0.56
3:L:8:ALA:HA	3:L:105:THR:HB	1.88	0.56
2:C:61:ALA:O	2:C:62:GLN:HB2	2.06	0.56
2:H:150:PHE:CD2	2:H:179:LEU:HD23	2.40	0.56
3:L:22:CYS:HB3	3:L:23:THR:CA	2.35	0.56
2:C:193:LEU:O	2:C:195:THR:N	2.38	0.56
1:B:64:ILE:HD13	1:B:72:VAL:HG21	1.87	0.56
3:L:9:SER:C	3:L:10:VAL:HG12	2.26	0.56
3:D:16:GLN:O	3:D:16:GLN:HG3	2.03	0.56
1:B:141:TYR:O	1:B:144:THR:HG22	2.07	0.55
1:B:215:HIS:CD2	1:B:227:HIS:HB3	2.41	0.55
2:H:6:GLN:H	2:H:109:GLN:NE2	2.03	0.55
2:H:131:SER:HG	2:H:133:LYS:CA	1.99	0.55
3:D:54:SER:HB3	3:D:66:GLY:O	2.07	0.55
3:D:124:SER:O	3:D:127:GLN:N	2.38	0.55
1:B:494:ALA:O	1:B:495:ARG:HB2	2.06	0.55
2:H:18:LEU:HD11	2:H:20:ILE:HG13	1.88	0.55
2:C:157:SER:HB3	2:C:201:ASN:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:16:GLN:HB2	3:D:17:SER:HB3	1.88	0.55
1:B:546:GLN:C	1:B:548:GLN:N	2.40	0.55
3:L:22:CYS:H	3:L:37:TRP:HH2	1.54	0.55
1:B:35:GLN:HG2	1:B:59:GLN:NE2	2.22	0.55
3:D:70:GLY:HA2	3:D:72:THR:N	2.22	0.55
1:B:559:ALA:HA	1:B:562:CYS:SG	2.47	0.55
3:L:6:GLN:HB2	3:L:7:PRO:HD2	1.88	0.55
3:D:50:ILE:HD13	3:D:53:VAL:O	2.06	0.55
1:A:1:THR:OG1	1:A:2:GLN:N	2.39	0.55
1:B:489:CYS:SG	1:B:498:CYS:N	2.80	0.55
2:H:38:ARG:HB3	2:H:48:MET:HE1	1.87	0.55
2:C:166:GLY:HA3	2:C:187:THR:HB	1.88	0.55
1:B:333:ALA:HB2	1:B:355:LEU:HG	1.88	0.55
1:B:503:PRO:HD2	1:B:504:THR:HG22	1.89	0.55
1:B:63:LEU:HD13	1:B:93:ALA:HB3	1.89	0.54
1:A:248:ALA:O	1:A:262:ASN:ND2	2.37	0.54
1:A:553:THR:HG23	6:A:1114:HOH:O	1.78	0.54
2:C:124:SER:HB3	2:C:126:PHE:CE2	2.42	0.54
2:C:159:ASN:OD1	2:C:199:ILE:N	2.41	0.54
3:D:70:GLY:HA2	3:D:72:THR:H	1.72	0.54
2:C:158:TRP:CZ3	2:C:198:TYR:HB3	2.39	0.54
1:B:249:LEU:O	1:B:262:ASN:N	2.40	0.54
3:D:123:PRO:CA	3:D:127:GLN:HE22	2.10	0.54
1:B:542:HIS:ND1	1:B:543:PRO:CD	2.71	0.54
1:B:557:PRO:HD2	1:B:561:GLN:NE2	2.22	0.54
3:L:50:ILE:HG22	3:L:56:ARG:HA	1.89	0.54
2:C:204:HIS:CE1	2:C:206:PRO:HB2	2.43	0.54
2:C:47:TRP:CZ2	2:C:49:GLY:HA2	2.43	0.54
1:B:542:HIS:CG	1:B:543:PRO:N	2.75	0.54
1:A:237:ASN:CG	4:E:1:NAG:C1	2.74	0.53
2:C:4:LEU:O	2:C:108:GLY:HA2	2.08	0.53
2:C:128:LEU:HD23	3:D:122:PRO:O	2.06	0.53
2:H:18:LEU:HD23	2:H:86:LEU:HD11	1.89	0.53
2:C:45:LEU:HG	3:D:89:TYR:CZ	2.44	0.53
2:C:189:PRO:CB	2:C:191:SER:HB3	2.26	0.53
1:A:554:CYS:SG	1:A:556:GLY:N	2.82	0.53
3:L:23:THR:CB	3:L:72:THR:OG1	2.55	0.53
1:A:450:THR:O	1:A:477:ARG:HB2	2.07	0.53
1:B:95:LEU:HD23	1:B:134:GLN:HB3	1.90	0.53
1:B:250:VAL:CG1	1:B:261:PRO:CA	2.57	0.53
1:B:183:TRP:N	1:B:189:ASP:O	2.31	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:159:ASN:N	2:C:199:ILE:O	2.35	0.52
3:D:6:GLN:HB2	3:D:105:THR:CG2	2.39	0.52
1:A:253:ASN:HD22	1:A:256:THR:HG1	1.51	0.52
1:A:443:LEU:HD23	1:A:469:GLN:HA	1.91	0.52
1:B:143:ASP:OD1	1:B:143:ASP:N	2.40	0.52
2:H:157:SER:OG	2:H:161:GLY:N	2.41	0.52
1:B:248:ALA:O	1:B:265:GLY:HA3	2.10	0.52
1:B:555:PHE:HB2	1:B:562:CYS:HA	1.90	0.52
1:B:35:GLN:HG2	1:B:59:GLN:HE21	1.74	0.52
1:B:249:LEU:HD11	1:B:287:GLY:HA2	1.92	0.52
3:L:200:THR:HG23	3:L:207:PRO:HD3	1.92	0.52
1:A:14:PRO:O	1:A:17:PRO:HD3	2.09	0.52
1:B:253:ASN:HB2	1:B:260:MET:HE3	1.90	0.52
1:B:262:ASN:O	1:B:264:GLU:N	2.38	0.52
2:C:39:GLN:OE1	3:D:40:GLN:NE2	2.37	0.52
3:D:72:THR:CA	3:D:73:ALA:CB	2.84	0.52
1:B:29:GLN:HA	1:B:51:PHE:HB2	1.92	0.52
1:B:128:LYS:HA	1:B:155:ASN:OD1	2.10	0.52
2:H:95:TYR:CE1	3:L:45:ALA:HB2	2.44	0.52
2:H:167:VAL:O	2:H:168:HIS:ND1	2.43	0.52
3:L:148:LYS:HB3	3:L:200:THR:HB	1.91	0.52
1:B:542:HIS:CE1	1:B:543:PRO:CD	2.81	0.52
1:B:542:HIS:ND1	1:B:543:PRO:N	2.57	0.52
2:C:142:LEU:HD13	6:C:306:HOH:O	2.09	0.52
2:C:193:LEU:O	2:C:195:THR:HB	2.10	0.52
3:D:47:LYS:HG3	3:D:48:LEU:N	2.24	0.52
3:D:164:GLU:OE1	3:D:178:LEU:HD21	2.10	0.52
2:H:2:VAL:HB	2:H:106:TYR:CE2	2.45	0.52
1:B:223:THR:O	1:B:223:THR:OG1	2.25	0.51
2:H:67:ARG:NH1	2:H:83:LEU:HD21	2.25	0.51
3:L:53:VAL:O	3:L:66:GLY:O	2.28	0.51
3:L:115:ALA:HB1	3:L:204:LEU:HG	1.92	0.51
2:C:185:VAL:HG21	3:D:138:LEU:HD22	1.91	0.51
3:D:145:ARG:HH21	3:D:166:VAL:HG11	1.76	0.51
1:A:533:VAL:HB	6:A:1111:HOH:O	2.10	0.51
3:D:37:TRP:HB2	3:D:50:ILE:H	1.75	0.51
1:A:444:ALA:HB3	1:A:471:LEU:HD23	1.93	0.51
3:L:49:MET:O	3:L:49:MET:HG2	2.09	0.51
1:B:140:CYS:HA	1:B:166:ARG:NH2	2.22	0.51
1:B:528:LEU:HB2	1:B:529:PRO:CD	2.35	0.51
1:B:209:LEU:HB2	1:B:212:ASP:OD2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:ASN:C	1:B:264:GLU:H	2.12	0.51
2:H:121:LYS:HG3	2:H:122:GLY:H	1.76	0.51
3:D:53:VAL:HG23	3:D:54:SER:N	2.26	0.50
3:D:71:ASN:N	3:D:71:ASN:OD1	2.40	0.50
3:D:123:PRO:HG2	3:D:127:GLN:HB3	1.93	0.50
2:C:64:LEU:HB3	2:C:68:VAL:HG22	1.93	0.50
2:C:123:PRO:HA	2:C:149:TYR:HB3	1.92	0.50
1:A:8:ASP:OD1	1:A:10:LYS:NZ	2.44	0.50
1:A:23:MET:HG3	1:A:419:TYR:OH	2.11	0.50
1:A:390:ILE:HG22	1:A:426:LEU:HD21	1.93	0.50
1:B:543:PRO:O	1:B:544:GLU:HB2	2.12	0.50
1:B:385:THR:O	1:B:385:THR:OG1	2.26	0.50
1:B:542:HIS:CG	1:B:543:PRO:HD2	2.43	0.50
3:L:83:GLU:HB3	6:L:301:HOH:O	2.12	0.50
2:C:73:ASP:OD1	2:C:75:SER:OG	2.28	0.50
3:D:124:SER:C	3:D:126:GLU:N	2.65	0.50
2:H:61:ALA:HB3	2:H:64:LEU:HB2	1.93	0.50
2:H:158:TRP:CH2	2:H:200:CYS:HB3	2.46	0.50
3:L:9:SER:O	3:L:10:VAL:HG12	2.10	0.50
3:D:135:VAL:HG12	3:D:151:TRP:CH2	2.46	0.50
1:A:560:ASP:HB3	1:A:561:GLN:OE1	2.11	0.50
1:B:546:GLN:CG	1:B:548:GLN:CD	2.79	0.50
2:H:205:LYS:HA	2:H:208:ASN:H	1.76	0.50
3:L:72:THR:CA	3:L:73:ALA:HB3	2.33	0.50
1:A:344:GLY:HA2	1:A:380:THR:OG1	2.11	0.50
1:B:2:GLN:HG3	1:B:3:VAL:HG23	1.94	0.50
1:B:29:GLN:O	1:B:29:GLN:HG3	2.07	0.50
1:B:290:THR:HB	1:B:292:VAL:H	1.77	0.50
3:L:9:SER:O	3:L:10:VAL:CG1	2.60	0.50
3:D:153:VAL:HG13	3:D:195:TYR:CE1	2.47	0.50
1:A:323:LEU:HD23	1:A:328:LEU:HD13	1.93	0.49
3:D:136:VAL:HG13	3:D:181:THR:HG22	1.93	0.49
1:A:524:VAL:HG12	1:A:532:TYR:HA	1.94	0.49
2:H:18:LEU:HB3	2:H:86:LEU:HD21	1.93	0.49
1:A:19:THR:HB	1:A:472:LEU:HD13	1.93	0.49
1:B:545:CYS:SG	1:B:564:ALA:HB3	2.53	0.49
3:L:10:VAL:HG23	3:L:18:ILE:HG22	1.94	0.49
1:B:284:THR:CG2	1:B:286:VAL:HG13	2.42	0.49
2:C:36:TRP:CZ2	2:C:81:MET:HB2	2.48	0.49
2:H:171:PRO:HD2	3:L:165:SER:HB3	1.93	0.49
1:A:64:ILE:O	1:A:94:VAL:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:ASN:ND2	4:E:1:NAG:C2	2.58	0.49
1:A:419:TYR:CE1	1:A:443:LEU:HD12	2.48	0.49
1:B:268:THR:C	1:B:269:PHE:O	2.48	0.49
3:D:154:ASP:HB2	3:D:192:HIS:ND1	2.28	0.49
2:C:188:VAL:HG11	2:C:198:TYR:CE1	2.46	0.49
1:B:146:LEU:HB2	1:B:181:ARG:CZ	2.43	0.49
1:A:319:VAL:HG21	1:A:349:PHE:HE1	1.78	0.48
2:H:4:LEU:HD22	2:H:22:CYS:SG	2.53	0.48
3:D:192:HIS:O	3:D:214:ARG:NH1	2.46	0.48
1:A:144:THR:O	1:A:181:ARG:HB3	2.13	0.48
1:A:237:ASN:ND2	4:E:1:NAG:N2	2.61	0.48
1:B:372:PRO:HB3	1:B:397:LEU:HD11	1.95	0.48
2:C:23:LYS:HG3	2:C:78:THR:OG1	2.13	0.48
1:B:278:PRO:HG2	1:B:281:TYR:CD1	2.48	0.48
1:B:446:ILE:HG13	1:B:471:LEU:HD21	1.95	0.48
2:C:33:TRP:HB2	2:C:99:GLU:OE2	2.13	0.48
2:C:36:TRP:CZ3	2:C:96:CYS:HB3	2.48	0.48
1:B:250:VAL:HA	1:B:260:MET:O	2.13	0.48
1:B:250:VAL:CA	1:B:262:ASN:H	2.22	0.48
2:C:2:VAL:HG21	2:C:106:TYR:CZ	2.49	0.48
1:B:353:ALA:HA	1:B:389:TYR:O	2.14	0.48
1:B:551:SER:O	1:B:552:VAL:O	2.32	0.48
3:D:135:VAL:HG23	3:D:184:LEU:HD12	1.96	0.48
1:A:335:THR:HG22	1:A:338:ASN:ND2	2.29	0.48
1:A:128:LYS:HA	1:A:155:ASN:OD1	2.14	0.48
1:A:360:ASP:OD1	1:A:360:ASP:N	2.47	0.48
3:L:21:SER:O	3:L:22:CYS:C	2.50	0.48
2:C:159:ASN:ND2	6:C:311:HOH:O	2.47	0.48
3:D:163:GLN:HG3	3:D:164:GLU:H	1.79	0.48
1:A:325:MET:O	1:A:329:ARG:N	2.47	0.47
1:A:528:LEU:HD23	1:A:528:LEU:H	1.77	0.47
1:B:18:GLU:HG3	1:B:474:THR:HG21	1.96	0.47
1:A:514:ARG:HD2	1:A:531:GLU:OE1	2.14	0.47
1:B:1:THR:HG23	1:B:468:HIS:NE2	2.30	0.47
3:D:50:ILE:HG22	3:D:56:ARG:HA	1.95	0.47
3:D:53:VAL:HG23	3:D:54:SER:H	1.78	0.47
1:A:99:ASP:HA	1:A:100:PRO:HD3	1.73	0.47
1:A:300:VAL:HG12	1:A:301:THR:N	2.29	0.47
3:D:188:ASP:HB3	6:D:301:HOH:O	2.14	0.47
2:H:44:GLY:HA2	3:L:89:TYR:OH	2.14	0.47
2:H:127:PRO:HB3	2:H:215:VAL:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:124:SER:HB3	2:C:126:PHE:CZ	2.50	0.47
1:A:489:CYS:SG	1:A:498:CYS:N	2.88	0.47
1:B:523:ARG:HD2	1:B:531:GLU:OE2	2.14	0.47
2:C:143:GLY:HA2	2:C:158:TRP:CZ2	2.49	0.47
3:D:45:ALA:HA	3:D:46:PRO:HD3	1.53	0.47
1:A:116:ARG:NH2	1:A:168:ARG:HH12	2.12	0.47
2:C:19:LYS:HG2	2:C:82:GLU:HB2	1.96	0.47
3:D:137:CYS:HB2	3:D:151:TRP:CZ2	2.49	0.47
1:B:524:VAL:HG12	1:B:532:TYR:HA	1.97	0.47
2:C:35:GLY:HA3	2:C:104:PHE:HE2	1.79	0.47
3:D:23:THR:HG22	3:D:72:THR:CG2	2.22	0.46
3:D:123:PRO:CD	3:D:124:SER:H	2.27	0.46
1:A:140:CYS:HB2	1:A:168:ARG:HH21	1.80	0.46
1:B:157:LEU:HD23	1:B:157:LEU:HA	1.63	0.46
1:B:119:GLN:OE1	1:B:121:ARG:NH2	2.49	0.46
1:B:144:THR:O	1:B:181:ARG:HB3	2.14	0.46
2:H:73:ASP:OD2	2:H:76:THR:HG23	2.16	0.46
3:L:23:THR:CG2	3:L:72:THR:OG1	2.63	0.46
3:L:72:THR:CA	3:L:73:ALA:CB	2.83	0.46
2:C:88:SER:HB2	2:C:89:ASP:HB3	1.97	0.46
3:D:6:GLN:HB3	3:D:21:SER:O	2.15	0.46
2:H:131:SER:HG	2:H:133:LYS:C	2.19	0.46
3:L:91:SER:HB3	3:L:101:PHE:CD1	2.50	0.46
2:C:168:HIS:HB3	6:D:316:HOH:O	2.15	0.46
3:D:17:SER:O	3:D:18:ILE:HG12	2.15	0.46
1:B:556:GLY:HA3	1:B:561:GLN:HG2	1.97	0.46
2:H:131:SER:C	2:H:133:LYS:N	2.58	0.46
3:D:68:LYS:HG2	3:D:69:SER:H	1.80	0.46
1:A:168:ARG:HB2	2:C:31:SER:HB3	1.97	0.46
1:B:11:LEU:HD23	1:B:11:LEU:HA	1.76	0.46
2:H:51:ILE:CG1	2:H:70:MET:HB2	2.45	0.46
2:C:91:THR:HA	2:C:113:VAL:O	2.15	0.46
2:C:130:PRO:CG	2:C:193:LEU:HD11	2.26	0.46
1:A:29:GLN:HA	1:A:51:PHE:HB2	1.98	0.46
3:L:80:LEU:HD11	3:L:107:LEU:HD21	1.98	0.46
2:C:163:LEU:HD22	6:C:311:HOH:O	2.15	0.46
1:B:466:ASN:O	1:B:469:GLN:HB2	2.16	0.46
2:H:130:PRO:HA	2:H:134:SER:OG	2.15	0.46
3:L:41:HIS:HB3	3:L:42:PRO:CD	2.44	0.46
3:D:20:ILE:HG22	3:D:21:SER:N	2.29	0.46
3:D:8:ALA:HA	3:D:105:THR:CA	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:148:LYS:HA	3:D:148:LYS:HE3	1.97	0.46
2:H:48:MET:HE1	2:H:94:TYR:CD2	2.51	0.45
3:L:8:ALA:HA	3:L:105:THR:CA	2.46	0.45
3:D:6:GLN:HE21	3:D:105:THR:HG23	1.81	0.45
3:D:64:PHE:CE1	3:D:77:ILE:HG12	2.51	0.45
3:D:78:SER:OG	3:D:79:GLY:N	2.48	0.45
1:A:404:GLN:O	1:A:435:SER:OG	2.34	0.45
3:D:17:SER:C	3:D:18:ILE:HG12	2.36	0.45
3:D:80:LEU:HA	3:D:80:LEU:HD13	1.54	0.45
1:A:186:SER:OG	1:A:187:SER:N	2.50	0.45
2:H:54:TYR:HD2	2:H:55:ASN:HD22	1.64	0.45
3:D:18:ILE:HG22	3:D:19:THR:N	2.27	0.45
1:A:517:GLU:HG3	1:A:518:CYS:N	2.27	0.45
1:A:529:PRO:C	1:A:530:ARG:HG3	2.37	0.45
1:B:226:LYS:HE2	1:B:226:LYS:HB3	1.64	0.45
2:H:18:LEU:HD12	2:H:19:LYS:N	2.31	0.45
2:C:121:LYS:NZ	6:C:305:HOH:O	2.50	0.45
2:C:150:PHE:CD2	2:C:179:LEU:HD23	2.52	0.45
3:D:123:PRO:O	3:D:127:GLN:NE2	2.49	0.45
1:A:238:HIS:CD2	1:A:238:HIS:C	2.90	0.45
1:B:146:LEU:N	1:B:191:GLN:OE1	2.40	0.45
1:A:221:GLY:C	1:A:231:LEU:HG	2.37	0.45
1:A:393:TRP:HB2	1:A:426:LEU:HD22	1.98	0.45
1:B:59:GLN:O	1:B:83:THR:HB	2.17	0.45
1:B:239:SER:HA	5:B:1001:NAG:H83	1.97	0.45
1:B:274:VAL:HG12	1:B:276:ALA:N	2.32	0.45
1:A:238:HIS:O	1:A:239:SER:HB2	2.17	0.45
1:A:528:LEU:N	1:A:528:LEU:CD2	2.73	0.45
1:A:554:CYS:O	1:A:555:PHE:CD1	2.70	0.45
1:B:38:LEU:HA	1:B:38:LEU:HD12	1.77	0.45
1:B:265:GLY:C	1:B:266:ARG:HG2	2.37	0.45
1:B:326:GLU:O	1:B:327:HIS:ND1	2.50	0.45
2:H:36:TRP:CZ3	2:H:96:CYS:HB3	2.51	0.45
2:H:152:GLU:O	2:H:206:PRO:HG2	2.16	0.45
2:H:167:VAL:C	2:H:168:HIS:HD1	2.21	0.45
2:C:173:VAL:O	2:C:180:TYR:HA	2.17	0.45
3:D:124:SER:O	3:D:126:GLU:N	2.50	0.45
1:A:13:LEU:HA	1:A:14:PRO:HD3	1.83	0.45
1:A:155:ASN:HD22	1:A:158:ALA:HB2	1.81	0.45
1:B:7:THR:O	1:B:37:ASN:HB2	2.16	0.45
3:L:17:SER:O	3:L:18:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:16:GLU:O	2:C:86:LEU:HB2	2.17	0.45
3:D:164:GLU:HA	3:D:179:SER:O	2.17	0.45
2:H:3:GLN:O	2:H:24:GLY:HA2	2.17	0.44
2:H:51:ILE:HG22	2:H:52:SER:O	2.16	0.44
1:A:140:CYS:HA	1:A:166:ARG:NH2	2.27	0.44
1:A:175:PRO:HB3	3:D:95:SER:HA	1.99	0.44
1:A:438:GLU:OE2	1:A:465:ARG:NH1	2.48	0.44
2:H:35:GLY:HA3	2:H:104:PHE:CE1	2.52	0.44
2:H:51:ILE:HD11	2:H:70:MET:O	2.16	0.44
2:C:188:VAL:HG21	2:C:198:TYR:CE1	2.52	0.44
3:L:63:ARG:HG2	3:L:78:SER:HB3	1.98	0.44
1:B:21:LEU:HD12	1:B:43:LEU:HD22	2.00	0.44
1:B:118:LEU:HD23	1:B:118:LEU:HA	1.69	0.44
1:B:186:SER:HB3	1:B:189:ASP:OD2	2.17	0.44
1:A:297:ASN:OD1	1:A:311:LYS:HG2	2.17	0.44
2:H:131:SER:C	2:H:133:LYS:H	2.03	0.44
2:C:129:ALA:HA	2:C:130:PRO:HD3	1.54	0.44
2:C:194:GLY:HA3	2:C:217:PRO:CG	2.45	0.44
1:A:238:HIS:CD2	1:A:238:HIS:O	2.70	0.44
1:B:293:CYS:HA	1:B:294:PRO:HD3	1.87	0.44
1:B:551:SER:O	1:B:552:VAL:C	2.55	0.44
3:L:13:SER:CA	3:L:110:LEU:HB2	2.40	0.44
2:C:33:TRP:O	2:C:34:ILE:HD12	2.17	0.44
3:D:22:CYS:CB	3:D:73:ALA:CB	2.61	0.44
2:C:185:VAL:HG11	3:D:138:LEU:HD22	2.00	0.44
1:B:116:ARG:HA	1:B:138:GLN:O	2.17	0.44
1:B:480:ASP:N	1:B:480:ASP:OD1	2.51	0.44
3:D:83:GLU:HG3	3:D:171:SER:HB2	2.00	0.44
1:A:41:THR:HA	1:A:65:ALA:O	2.17	0.44
1:B:553:THR:CG2	1:B:554:CYS:N	2.48	0.44
2:H:216:GLU:H	2:H:216:GLU:HG2	1.61	0.44
3:L:8:ALA:HA	3:L:105:THR:HA	1.99	0.44
1:A:319:VAL:HG22	1:A:320:CYS:N	2.33	0.43
1:A:353:ALA:HA	1:A:389:TYR:O	2.17	0.43
1:B:119:GLN:HA	1:B:183:TRP:HB3	2.00	0.43
2:C:90:ASP:O	2:C:94:TYR:HE1	2.01	0.43
2:C:150:PHE:HE2	2:C:178:GLY:O	2.01	0.43
2:C:204:HIS:O	2:C:207:SER:N	2.50	0.43
1:B:404:GLN:OE1	1:B:434:ARG:NH1	2.51	0.43
3:D:172:LYS:HA	3:D:172:LYS:HD2	1.93	0.43
1:A:238:HIS:CB	1:A:273:CYS:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:12:LYS:O	2:H:115:VAL:HA	2.18	0.43
2:H:158:TRP:CZ3	2:H:200:CYS:HB3	2.53	0.43
1:A:7:THR:O	1:A:37:ASN:HB2	2.18	0.43
1:A:401:SER:O	1:A:404:GLN:N	2.49	0.43
1:A:438:GLU:HB2	1:A:465:ARG:NH1	2.34	0.43
1:B:116:ARG:NH2	1:B:168:ARG:HH12	2.17	0.43
3:L:28:ASP:O	3:L:92:SER:OG	2.36	0.43
2:C:3:GLN:HB2	2:C:25:SER:OG	2.18	0.43
3:D:6:GLN:HB2	3:D:105:THR:HG23	2.00	0.43
4:E:2:NAG:C1	4:E:2:NAG:C8	2.96	0.43
1:A:215:HIS:CD2	1:A:227:HIS:HB3	2.53	0.43
1:A:374:GLN:O	1:A:377:VAL:HG13	2.18	0.43
1:B:219:ALA:HB2	1:B:234:LEU:HA	2.01	0.43
2:H:131:SER:OG	2:H:133:LYS:C	2.52	0.43
3:L:7:PRO:O	3:L:8:ALA:HB3	2.17	0.43
2:C:13:LYS:NZ	6:C:302:HOH:O	2.39	0.43
1:A:477:ARG:HA	1:A:478:PRO:HD3	1.83	0.43
1:B:70:ARG:HA	1:B:114:GLY:O	2.18	0.43
3:L:107:LEU:HD12	3:L:108:THR:N	2.32	0.43
2:C:36:TRP:HB3	2:C:48:MET:HE3	2.00	0.43
2:C:148:ASP:HA	2:C:179:LEU:HB2	2.00	0.43
1:B:34:VAL:O	1:B:34:VAL:HG22	2.18	0.43
1:B:43:LEU:HD13	1:B:49:LEU:HD21	2.00	0.43
1:B:555:PHE:HB3	1:B:561:GLN:O	2.18	0.43
3:L:5:THR:O	3:L:23:THR:N	2.52	0.43
2:C:6:GLN:O	2:C:109:GLN:NE2	2.52	0.43
2:C:143:GLY:HA2	2:C:158:TRP:CH2	2.53	0.43
1:A:527:GLY:HA2	1:A:528:LEU:HD23	2.01	0.43
1:B:361:GLY:HA2	1:B:369:PRO:HG3	2.00	0.43
1:B:442:GLY:O	1:B:469:GLN:HG2	2.18	0.43
3:L:91:SER:HB3	3:L:101:PHE:CE1	2.54	0.43
3:D:164:GLU:HG2	3:D:178:LEU:HD21	2.01	0.43
1:A:347:LYS:HD2	1:A:383:GLU:OE2	2.19	0.43
1:B:301:THR:HG23	1:B:306:THR:O	2.18	0.43
2:C:199:ILE:HG12	2:C:214:LYS:CB	2.48	0.43
2:C:209:THR:O	2:C:211:VAL:HG23	2.19	0.43
3:D:138:LEU:C	3:D:139:LEU:HD12	2.39	0.43
1:B:7:THR:C	1:B:39:GLU:OE1	2.57	0.43
3:L:14:PRO:HD3	3:L:110:LEU:N	2.29	0.43
1:A:249:LEU:HD11	1:A:267:TYR:CE2	2.54	0.42
1:A:464:PHE:CE2	1:A:470:ALA:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:LYS:HG2	1:B:229:ASP:OD2	2.19	0.42
1:B:366:ASN:ND2	6:B:1113:HOH:O	2.45	0.42
2:H:124:SER:HB3	2:H:126:PHE:CZ	2.54	0.42
2:H:150:PHE:CD1	2:H:151:PRO:HA	2.54	0.42
3:L:66:GLY:HA3	3:L:75:LEU:HA	2.00	0.42
1:A:178:LYS:H	1:A:178:LYS:HG3	1.32	0.42
2:H:33:TRP:HB2	2:H:99:GLU:OE2	2.20	0.42
3:L:68:LYS:HB3	3:L:73:ALA:H	1.84	0.42
3:D:153:VAL:HG13	3:D:195:TYR:HE1	1.84	0.42
1:B:175:PRO:HD3	3:L:93:TYR:OH	2.20	0.42
1:B:453:CYS:SG	1:B:477:ARG:HG2	2.58	0.42
1:B:546:GLN:CG	1:B:548:GLN:NE2	2.77	0.42
3:L:184:LEU:HD13	3:L:189:TYR:HD1	1.85	0.42
1:B:115:LEU:HD21	1:B:118:LEU:HD23	2.00	0.42
2:C:140:ALA:HB2	2:C:190:SER:HB3	2.01	0.42
2:C:194:GLY:N	2:C:217:PRO:HD2	2.33	0.42
3:D:151:TRP:CZ3	3:D:197:CYS:HB2	2.54	0.42
1:A:81:ARG:HG2	1:A:127:LEU:HD12	2.00	0.42
1:B:546:GLN:HG2	1:B:546:GLN:O	2.19	0.42
2:C:67:ARG:NH1	2:C:90:ASP:OD2	2.53	0.42
2:C:120:THR:OG1	2:C:151:PRO:HD3	2.19	0.42
2:C:186:VAL:HG22	2:C:188:VAL:HG13	2.00	0.42
3:D:154:ASP:OD1	3:D:193:LYS:N	2.53	0.42
1:A:164:THR:HG22	1:A:166:ARG:HH12	1.84	0.42
1:B:546:GLN:CD	1:B:548:GLN:CG	2.85	0.42
1:B:423:LEU:HB2	1:B:446:ILE:HG23	2.00	0.42
3:L:121:PHE:HA	3:L:122:PRO:HD2	1.84	0.42
2:C:132:SER:HA	2:C:135:THR:HG23	2.02	0.42
2:C:143:GLY:HA3	2:C:184:SER:O	2.19	0.42
1:A:157:LEU:HD23	1:A:157:LEU:HA	1.84	0.42
3:L:8:ALA:HA	3:L:106:LYS:N	2.33	0.42
3:L:9:SER:C	3:L:10:VAL:CG1	2.87	0.42
3:D:94:THR:C	3:D:96:SER:H	2.23	0.42
3:D:131:GLY:CA	3:D:186:LYS:HB2	2.30	0.42
2:H:6:GLN:HE21	2:H:6:GLN:HB3	1.73	0.42
1:B:250:VAL:HG12	1:B:261:PRO:N	2.26	0.42
1:B:321:TYR:CD2	1:B:326:GLU:HB3	2.54	0.42
1:B:509:CYS:SG	1:B:511:GLN:O	2.77	0.42
2:H:64:LEU:HB3	2:H:68:VAL:CG2	2.47	0.42
1:A:175:PRO:HG2	3:D:97:SER:OG	2.20	0.41
1:B:72:VAL:HA	1:B:73:PRO:HD2	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:8:ALA:N	3:L:105:THR:HG22	2.34	0.41
3:L:51:TYR:CE2	3:L:55:LYS:HD2	2.55	0.41
1:B:407:GLN:O	1:B:437:ARG:HG2	2.20	0.41
1:B:532:TYR:CZ	1:B:539:LEU:HB2	2.55	0.41
3:L:38:TYR:N	3:L:89:TYR:O	2.53	0.41
3:L:122:PRO:HB3	3:L:212:PHE:CE1	2.55	0.41
2:C:47:TRP:CG	3:D:99:LEU:HB3	2.55	0.41
2:C:90:ASP:O	2:C:91:THR:C	2.58	0.41
2:C:193:LEU:HG	2:C:194:GLY:H	1.84	0.41
3:D:37:TRP:CD2	3:D:75:LEU:HB2	2.55	0.41
1:B:480:ASP:C	1:B:482:CYS:H	2.23	0.41
2:H:183:SER:OG	2:H:184:SER:N	2.54	0.41
3:L:7:PRO:O	3:L:8:ALA:CB	2.69	0.41
2:C:64:LEU:O	2:C:67:ARG:HB2	2.20	0.41
2:C:140:ALA:HB2	2:C:190:SER:CB	2.50	0.41
3:D:131:GLY:C	3:D:186:LYS:H	2.24	0.41
1:A:163:ASP:OD1	1:A:164:THR:N	2.54	0.41
1:A:266:ARG:HH11	1:A:266:ARG:CG	2.31	0.41
1:A:463:LEU:N	1:A:463:LEU:HD12	2.36	0.41
3:D:178:LEU:HD23	3:D:179:SER:N	2.35	0.41
1:A:384:ILE:CG2	1:A:386:GLY:O	2.51	0.41
1:B:426:LEU:N	1:B:449:ASN:OD1	2.29	0.41
1:A:525:LEU:HB2	1:A:526:GLN:HG3	2.01	0.41
1:B:445:LEU:HD12	1:B:472:LEU:O	2.20	0.41
2:H:18:LEU:HB3	2:H:86:LEU:CD2	2.51	0.41
2:H:88:SER:HB2	2:H:89:ASP:H	1.44	0.41
2:H:186:VAL:HG22	2:H:187:THR:H	1.86	0.41
3:L:156:ALA:O	3:L:158:GLN:HG2	2.20	0.41
3:L:166:VAL:HG23	3:L:177:SER:O	2.21	0.41
2:C:105:ASP:C	3:D:48:LEU:HD22	2.41	0.41
3:D:75:LEU:HD12	3:D:76:THR:H	1.84	0.41
1:A:79:ILE:HB	1:A:125:GLU:HB3	2.02	0.41
1:A:209:LEU:HB2	1:A:211:THR:HG22	2.02	0.41
1:B:513:LEU:HD22	1:B:515:GLY:O	2.20	0.41
3:L:139:LEU:HD13	3:L:178:LEU:HB3	2.03	0.41
3:D:23:THR:HG21	3:D:72:THR:HG21	2.02	0.41
3:D:139:LEU:O	3:D:177:SER:HA	2.20	0.41
1:B:18:GLU:CD	1:B:18:GLU:H	2.23	0.41
1:B:323:LEU:HB2	1:B:351:SER:O	2.20	0.41
2:H:34:ILE:HA	2:H:34:ILE:HD12	1.86	0.41
3:L:8:ALA:CA	3:L:105:THR:HB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:10:VAL:HG13	3:L:107:LEU:HD13	2.03	0.41
3:L:80:LEU:HD13	3:L:80:LEU:HA	1.77	0.41
2:C:18:LEU:HD22	2:C:113:VAL:HG11	2.03	0.41
2:C:142:LEU:HD22	2:C:193:LEU:HD11	1.98	0.41
2:C:155:THR:HB	2:C:203:ASN:HB3	2.03	0.41
2:C:166:GLY:HA3	2:C:187:THR:O	2.21	0.41
3:D:49:MET:HA	3:D:50:ILE:HA	1.86	0.41
1:A:340:GLN:H	1:A:340:GLN:HG2	1.43	0.41
1:A:352:LEU:HD12	1:A:384:ILE:CD1	2.50	0.41
1:A:378:PHE:O	1:A:381:LEU:HB3	2.21	0.41
2:H:131:SER:OG	2:H:134:SER:N	2.54	0.41
3:D:213:ASN:HB2	3:D:216:GLU:CD	2.41	0.41
1:A:319:VAL:HG21	1:A:349:PHE:CE1	2.56	0.40
1:B:492:LEU:HD11	1:B:520:GLU:OE1	2.22	0.40
2:C:105:ASP:O	3:D:48:LEU:HD22	2.21	0.40
2:C:1:GLU:O	2:C:26:GLY:HA3	2.22	0.40
1:A:175:PRO:HD3	3:D:93:TYR:OH	2.22	0.40
1:A:443:LEU:HB3	1:A:470:ALA:O	2.21	0.40
1:B:397:LEU:H	1:B:397:LEU:HG	1.76	0.40
1:B:546:GLN:CD	1:B:548:GLN:HB2	2.38	0.40
2:C:151:PRO:HD2	2:C:206:PRO:CB	2.49	0.40
1:A:80:VAL:HG22	1:A:126:ILE:HG12	2.03	0.40
1:A:155:ASN:ND2	1:A:158:ALA:HB2	2.36	0.40
2:H:98:ARG:O	2:H:104:PHE:HA	2.22	0.40
2:H:100:GLY:N	2:H:103:ALA:O	2.43	0.40
3:D:67:SER:O	3:D:74:SER:HB2	2.22	0.40
1:A:82:GLY:HA3	1:A:128:LYS:O	2.22	0.40
1:B:51:PHE:CD1	1:B:52:LEU:HD13	2.56	0.40
2:H:131:SER:HG	2:H:134:SER:N	2.20	0.40
3:L:8:ALA:O	3:L:9:SER:CB	2.69	0.40
2:C:39:GLN:O	2:C:93:VAL:HG23	2.22	0.40
3:D:38:TYR:HD1	3:D:48:LEU:HA	1.87	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:THR:O	2:C:191:SER:O[1_654]	1.78	0.42
1:B:160:THR:C	2:C:191:SER:O[1_654]	2.02	0.18
1:B:532:TYR:OH	2:H:195:THR:O[1_566]	2.11	0.09

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	551/564 (98%)	453 (82%)	86 (16%)	12 (2%)	6	27
1	B	551/564 (98%)	445 (81%)	90 (16%)	16 (3%)	4	22
2	C	215/217 (99%)	176 (82%)	35 (16%)	4 (2%)	8	31
2	H	215/217 (99%)	192 (89%)	18 (8%)	5 (2%)	6	26
3	D	215/217 (99%)	164 (76%)	41 (19%)	10 (5%)	2	13
3	L	215/217 (99%)	165 (77%)	43 (20%)	7 (3%)	4	19
All	All	1962/1996 (98%)	1595 (81%)	313 (16%)	54 (3%)	5	23

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	528	LEU
1	A	530	ARG
1	A	555	PHE
1	B	262	ASN
1	B	528	LEU
1	B	545	CYS
1	B	546	GLN
1	B	548	GLN
1	B	550	GLY
1	B	552	VAL
1	B	553	THR
1	B	554	CYS
1	B	555	PHE
2	H	151	PRO
3	L	9	SER
3	L	10	VAL
3	L	73	ALA
2	C	130	PRO
2	C	194	GLY
3	D	53	VAL

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Mol	Chain	Res	Type
3	D	68	LYS
3	D	123	PRO
3	D	124	SER
1	A	327	HIS
1	A	529	PRO
1	B	542	HIS
1	B	544	GLU
1	B	547	PRO
2	H	131	SER
3	L	7	PRO
2	C	195	THR
3	D	16	GLN
3	D	17	SER
3	D	73	ALA
3	D	125	ASP
1	A	239	SER
1	A	554	CYS
3	L	8	ALA
3	L	95	SER
2	C	193	LEU
3	D	95	SER
1	A	552	VAL
1	A	305	GLY
1	A	485	GLU
1	B	263	PRO
3	D	122	PRO
1	A	100	PRO
1	B	264	GLU
2	H	130	PRO
2	H	205	LYS
1	B	73	PRO
2	H	152	GLU
1	A	247	PRO
3	L	144	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	478/485 (99%)	401 (84%)	77 (16%)	2 10
1	B	478/485 (99%)	404 (84%)	74 (16%)	2 11
2	C	180/181 (99%)	149 (83%)	31 (17%)	2 8
2	H	180/181 (99%)	155 (86%)	25 (14%)	3 14
3	D	185/186 (100%)	144 (78%)	41 (22%)	1 3
3	L	185/186 (100%)	152 (82%)	33 (18%)	2 7
All	All	1686/1704 (99%)	1405 (83%)	281 (17%)	2 9

All (281) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	9	MET
1	A	13	LEU
1	A	18	GLU
1	A	35	GLN
1	A	45	THR
1	A	46	ASN
1	A	50	SER
1	A	52	LEU
1	A	69	VAL
1	A	74	LEU
1	A	78	ARG
1	A	80	VAL
1	A	134	GLN
1	A	153	LYS
1	A	156	GLN
1	A	159	LEU
1	A	160	THR
1	A	164	THR
1	A	178	LYS
1	A	181	ARG
1	A	192	SER
1	A	194	THR
1	A	206	LYS
1	A	216	GLU
1	A	223	THR
1	A	227	HIS
1	A	228	SER
1	A	238	HIS
1	A	247	PRO

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Mol	Chain	Res	Type
1	A	250	VAL
1	A	256	THR
1	A	260	MET
1	A	264	GLU
1	A	266	ARG
1	A	272	SER
1	A	282	LEU
1	A	283	SER
1	A	284	THR
1	A	286	VAL
1	A	290	THR
1	A	295	LEU
1	A	298	GLN
1	A	312	CYS
1	A	318	ARG
1	A	320	CYS
1	A	329	ARG
1	A	335	THR
1	A	360	ASP
1	A	367	THR
1	A	382	GLU
1	A	396	SER
1	A	435	SER
1	A	443	LEU
1	A	450	THR
1	A	457	THR
1	A	471	LEU
1	A	474	THR
1	A	480	ASP
1	A	485	GLU
1	A	487	LEU
1	A	504	THR
1	A	505	GLN
1	A	509	CYS
1	A	511	GLN
1	A	513	LEU
1	A	517	GLU
1	A	525	LEU
1	A	528	LEU
1	A	529	PRO
1	A	530	ARG
1	A	533	VAL

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Mol	Chain	Res	Type
1	A	546	GLN
1	A	549	ASN
1	A	553	THR
1	A	555	PHE
1	A	561	GLN
1	B	9	MET
1	B	13	LEU
1	B	21	LEU
1	B	32	GLN
1	B	34	VAL
1	B	35	GLN
1	B	45	THR
1	B	50	SER
1	B	52	LEU
1	B	69	VAL
1	B	83	THR
1	B	133	ILE
1	B	144	THR
1	B	156	GLN
1	B	160	THR
1	B	165	ASN
1	B	167	SER
1	B	181	ARG
1	B	195	ARG
1	B	206	LYS
1	B	213	CYS
1	B	216	GLU
1	B	223	THR
1	B	227	HIS
1	B	228	SER
1	B	256	THR
1	B	259	SER
1	B	272	SER
1	B	275	THR
1	B	282	LEU
1	B	284	THR
1	B	286	VAL
1	B	290	THR
1	B	295	LEU
1	B	298	GLN
1	B	312	CYS
1	B	314	LYS

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Mol	Chain	Res	Type
1	B	316	CYS
1	B	318	ARG
1	B	320	CYS
1	B	327	HIS
1	B	338	ASN
1	B	367	THR
1	B	380	THR
1	B	382	GLU
1	B	395	ASP
1	B	396	SER
1	B	401	SER
1	B	409	ILE
1	B	420	SER
1	B	422	THR
1	B	450	THR
1	B	465	ARG
1	B	471	LEU
1	B	480	ASP
1	B	481	GLU
1	B	485	GLU
1	B	491	GLN
1	B	492	LEU
1	B	504	THR
1	B	505	GLN
1	B	508	ASN
1	B	513	LEU
1	B	525	LEU
1	B	526	GLN
1	B	528	LEU
1	B	533	VAL
1	B	545	CYS
1	B	549	ASN
1	B	551	SER
1	B	554	CYS
1	B	555	PHE
1	B	558	GLU
1	B	561	GLN
2	H	10	GLU
2	H	18	LEU
2	H	34	ILE
2	H	43	GLN
2	H	50	TRP

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Mol	Chain	Res	Type
2	H	64	LEU
2	H	68	VAL
2	H	70	MET
2	H	86	LEU
2	H	88	SER
2	H	91	THR
2	H	130	PRO
2	H	132	SER
2	H	134	SER
2	H	142	LEU
2	H	147	LYS
2	H	149	TYR
2	H	150	PHE
2	H	152	GLU
2	H	154	VAL
2	H	155	THR
2	H	163	LEU
2	H	173	VAL
2	H	182	LEU
2	H	216	GLU
3	L	2	SER
3	L	13	SER
3	L	25	THR
3	L	36	SER
3	L	48	LEU
3	L	49	MET
3	L	63	ARG
3	L	65	SER
3	L	68	LYS
3	L	69	SER
3	L	71	ASN
3	L	74	SER
3	L	76	THR
3	L	80	LEU
3	L	87	ASP
3	L	96	SER
3	L	108	THR
3	L	109	VAL
3	L	110	LEU
3	L	120	ILE
3	L	125	ASP
3	L	129	LYS

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Mol	Chain	Res	Type
3	L	146	GLU
3	L	150	GLN
3	L	161	ASN
3	L	163	GLN
3	L	181	THR
3	L	186	LYS
3	L	202	GLN
3	L	205	SER
3	L	208	VAL
3	L	209	THR
3	L	212	PHE
2	C	2	VAL
2	C	11	VAL
2	C	19	LYS
2	C	21	SER
2	C	39	GLN
2	C	43	GLN
2	C	50	TRP
2	C	51	ILE
2	C	55	ASN
2	C	68	VAL
2	C	69	THR
2	C	70	MET
2	C	83	LEU
2	C	86	LEU
2	C	87	ARG
2	C	112	LEU
2	C	117	SER
2	C	142	LEU
2	C	145	LEU
2	C	148	ASP
2	C	150	PHE
2	C	152	GLU
2	C	159	ASN
2	C	173	VAL
2	C	179	LEU
2	C	182	LEU
2	C	184	SER
2	C	188	VAL
2	C	195	THR
2	C	212	ASP
2	C	215	VAL

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Mol	Chain	Res	Type
3	D	13	SER
3	D	22	CYS
3	D	25	THR
3	D	27	SER
3	D	28	ASP
3	D	29	VAL
3	D	36	SER
3	D	47	LYS
3	D	48	LEU
3	D	58	SER
3	D	63	ARG
3	D	65	SER
3	D	71	ASN
3	D	76	THR
3	D	80	LEU
3	D	85	GLU
3	D	90	CYS
3	D	97	SER
3	D	113	VAL
3	D	120	ILE
3	D	123	PRO
3	D	125	ASP
3	D	129	LYS
3	D	132	THR
3	D	137	CYS
3	D	138	LEU
3	D	146	GLU
3	D	148	LYS
3	D	154	ASP
3	D	158	GLN
3	D	159	SER
3	D	162	SER
3	D	163	GLN
3	D	164	GLU
3	D	166	VAL
3	D	167	THR
3	D	179	SER
3	D	185	SER
3	D	188	ASP
3	D	202	GLN
3	D	212	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	237	ASN
1	A	238	HIS
1	A	327	HIS
1	A	542	HIS
1	B	20	HIS
1	B	59	GLN
1	B	237	ASN
1	B	298	GLN
1	B	546	GLN
1	B	548	GLN
2	C	57	ASN
2	C	203	ASN
3	D	127	GLN
3	D	155	ASN
3	D	169	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

2 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	E	1	4,1	14,14,15	0.38	0	17,19,21	0.72	1 (5%)
4	NAG	E	2	4	14,14,15	0.48	0	17,19,21	1.84	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	E	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	2	NAG	C1-O5-C5	6.15	120.42	112.19
4	E	2	NAG	C4-C3-C2	3.06	115.50	111.02
4	E	2	NAG	O5-C1-C2	2.04	114.44	111.29
4	E	1	NAG	C3-C4-C5	2.02	113.89	110.23

There are no chirality outliers.

All (7) torsion outliers are listed below:

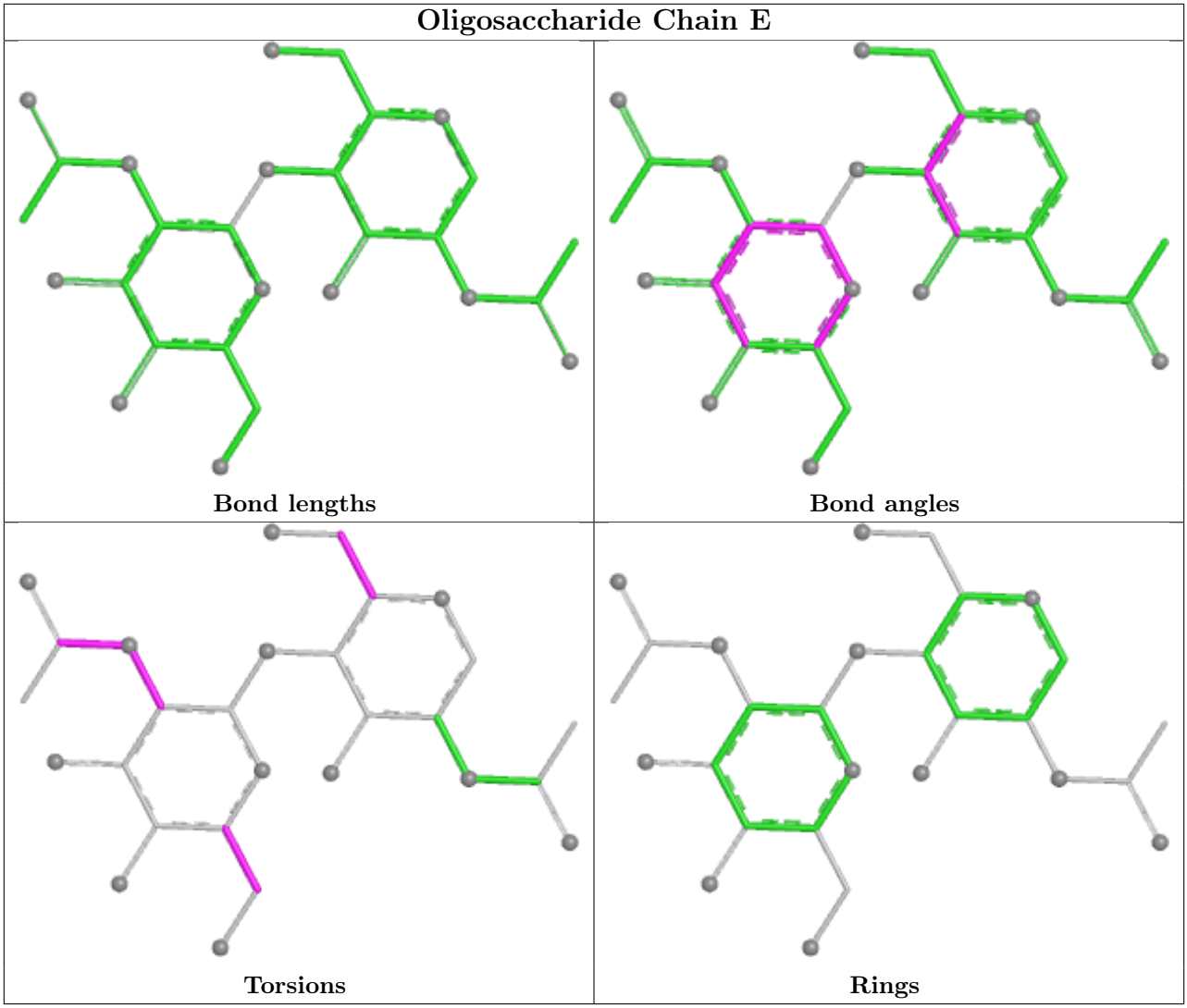
Mol	Chain	Res	Type	Atoms
4	E	2	NAG	C3-C2-N2-C7
4	E	2	NAG	C8-C7-N2-C2
4	E	2	NAG	O7-C7-N2-C2
4	E	2	NAG	O5-C5-C6-O6
4	E	1	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
4	E	1	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	2	NAG	2	0
4	E	1	NAG	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	NAG	B	1001	1	14,14,15	0.37	0	17,19,21	0.72	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1001	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1001	NAG	C8-C7-N2-C2
5	B	1001	NAG	O7-C7-N2-C2
5	B	1001	NAG	C4-C5-C6-O6
5	B	1001	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1001	NAG	10	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	555/564 (98%)	-0.23	15 (2%) 54 29	28, 52, 125, 178	0
1	B	555/564 (98%)	-0.26	9 (1%) 72 51	31, 54, 122, 152	0
2	C	217/217 (100%)	1.15	53 (24%) 0 0	39, 86, 170, 180	0
2	H	217/217 (100%)	0.05	9 (4%) 37 18	38, 70, 129, 178	0
3	D	217/217 (100%)	1.60	73 (33%) 0 0	45, 114, 187, 203	0
3	L	217/217 (100%)	0.34	22 (10%) 7 2	36, 102, 163, 185	0
All	All	1978/1996 (99%)	0.21	181 (9%) 9 3	28, 63, 166, 203	0

All (181) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	147	ALA	16.8
2	C	138	GLY	16.4
3	D	120	ILE	13.3
3	D	189	TYR	12.9
2	C	142	LEU	12.2
2	H	137	GLY	11.7
2	C	141	ALA	10.8
1	A	559	ALA	10.6
2	C	176	SER	10.0
2	C	125	VAL	9.7
3	D	159	SER	9.4
2	H	135	THR	9.1
2	C	130	PRO	9.1
2	C	140	ALA	8.0
2	C	164	THR	7.8
3	D	196	ALA	7.8
3	D	137	CYS	7.8
3	D	180	SER	7.6
2	H	136	SER	7.5

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Mol	Chain	Res	Type	RSRZ
3	D	209	THR	7.3
3	D	213	ASN	7.2
3	D	118	VAL	7.1
1	B	564	ALA	7.1
2	C	139	THR	7.0
2	C	126	PHE	7.0
2	C	168	HIS	6.9
1	A	547	PRO	6.7
3	D	190	GLU	6.4
3	D	195	TYR	6.4
3	D	124	SER	6.3
2	C	197	THR	6.3
2	C	137	GLY	6.2
3	D	157	LEU	6.1
2	C	190	SER	6.0
2	C	129	ALA	6.0
2	C	177	SER	5.8
3	D	149	VAL	5.8
2	C	178	GLY	5.7
3	L	156	ALA	5.6
3	D	151	TRP	5.6
2	C	192	SER	5.5
2	C	185	VAL	5.5
3	D	206	SER	5.3
3	D	205	SER	5.3
3	D	194	VAL	5.3
3	D	161	ASN	5.2
3	D	199	VAL	5.1
3	D	202	GLN	5.1
3	D	187	ALA	5.0
2	C	175	GLN	5.0
3	D	214	ARG	5.0
2	C	214	LYS	4.9
1	A	544	GLU	4.9
2	H	134	SER	4.9
1	A	543	PRO	4.8
3	D	200	THR	4.8
3	D	201	HIS	4.7
3	D	119	PHE	4.7
3	D	156	ALA	4.7
3	D	134	SER	4.6
3	D	188	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	541	CYS	4.5
1	A	548	GLN	4.5
3	L	197	CYS	4.4
2	C	201	ASN	4.4
1	A	540	PRO	4.3
3	D	160	GLY	4.3
3	L	199	VAL	4.3
1	B	563	VAL	4.3
3	D	197	CYS	4.2
3	D	138	LEU	4.2
2	C	128	LEU	4.2
3	D	185	SER	4.1
3	D	129	LYS	4.0
3	L	198	GLU	4.0
2	C	179	LEU	4.0
3	D	204	LEU	4.0
3	D	155	ASN	4.0
3	L	185	SER	4.0
1	B	550	GLY	4.0
2	H	138	GLY	3.9
3	L	157	LEU	3.9
3	D	207	PRO	3.9
1	A	542	HIS	3.9
2	C	196	GLN	3.9
3	D	117	SER	3.8
2	C	145	LEU	3.7
2	C	212	ASP	3.6
3	D	181	THR	3.5
3	D	186	LYS	3.5
3	L	195	TYR	3.5
1	A	528	LEU	3.4
2	C	217	PRO	3.4
3	D	148	LYS	3.4
3	D	165	SER	3.4
3	D	191	LYS	3.3
3	D	136	VAL	3.3
3	L	184	LEU	3.3
2	C	188	VAL	3.3
3	L	200	THR	3.3
3	D	203	GLY	3.3
3	L	152	LYS	3.2
2	C	165	SER	3.2

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Mol	Chain	Res	Type	RSRZ
3	D	215	GLY	3.2
2	C	173	VAL	3.2
3	D	198	GLU	3.1
2	C	143	GLY	3.1
3	D	114	ALA	3.1
3	L	155	ASN	3.1
3	L	196	ALA	3.1
2	C	187	THR	3.0
3	L	18	ILE	3.0
3	L	151	TRP	3.0
3	D	158	GLN	3.0
1	B	560	ASP	3.0
2	H	123	PRO	2.9
3	D	10	VAL	2.9
3	D	174	SER	2.8
3	L	153	VAL	2.8
2	C	134	SER	2.8
3	D	116	PRO	2.8
3	D	164	GLU	2.7
1	B	315	PRO	2.7
1	A	560	ASP	2.7
3	D	211	SER	2.7
2	C	203	ASN	2.7
3	D	78	SER	2.6
2	C	169	THR	2.6
2	C	210	LYS	2.6
2	C	211	VAL	2.6
3	D	146	GLU	2.6
2	C	146	VAL	2.6
2	C	183	SER	2.6
3	D	125	ASP	2.6
1	A	564	ALA	2.6
3	L	147	ALA	2.5
3	D	172	LYS	2.5
3	L	133	ALA	2.5
3	L	191	LYS	2.5
2	C	163	LEU	2.5
2	C	160	SER	2.5
3	L	186	LYS	2.5
2	C	133	LYS	2.5
1	A	254	THR	2.4
2	C	132	SER	2.4

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Mol	Chain	Res	Type	RSRZ
3	D	184	LEU	2.4
3	D	123	PRO	2.4
2	C	186	VAL	2.4
2	C	191	SER	2.4
3	D	126	GLU	2.4
1	A	513	LEU	2.4
2	C	167	VAL	2.4
3	D	150	GLN	2.3
3	D	152	LYS	2.3
2	H	120	THR	2.3
2	C	127	PRO	2.3
3	D	82	ALA	2.3
3	L	149	VAL	2.3
3	L	150	GLN	2.3
2	H	209	THR	2.2
1	B	562	CYS	2.2
3	D	217	CYS	2.2
1	B	1	THR	2.2
3	D	183	THR	2.2
1	B	313	SER	2.2
2	C	184	SER	2.2
3	L	188	ASP	2.2
2	C	161	GLY	2.2
2	C	123	PRO	2.2
2	C	144	CYS	2.2
3	D	212	PHE	2.1
3	D	208	VAL	2.1
3	D	127	GLN	2.1
3	D	163	GLN	2.1
2	H	139	THR	2.1
1	A	313	SER	2.1
1	A	545	CYS	2.1
1	B	296	HIS	2.1
3	D	121	PHE	2.0
2	C	195	THR	2.0
3	D	171	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

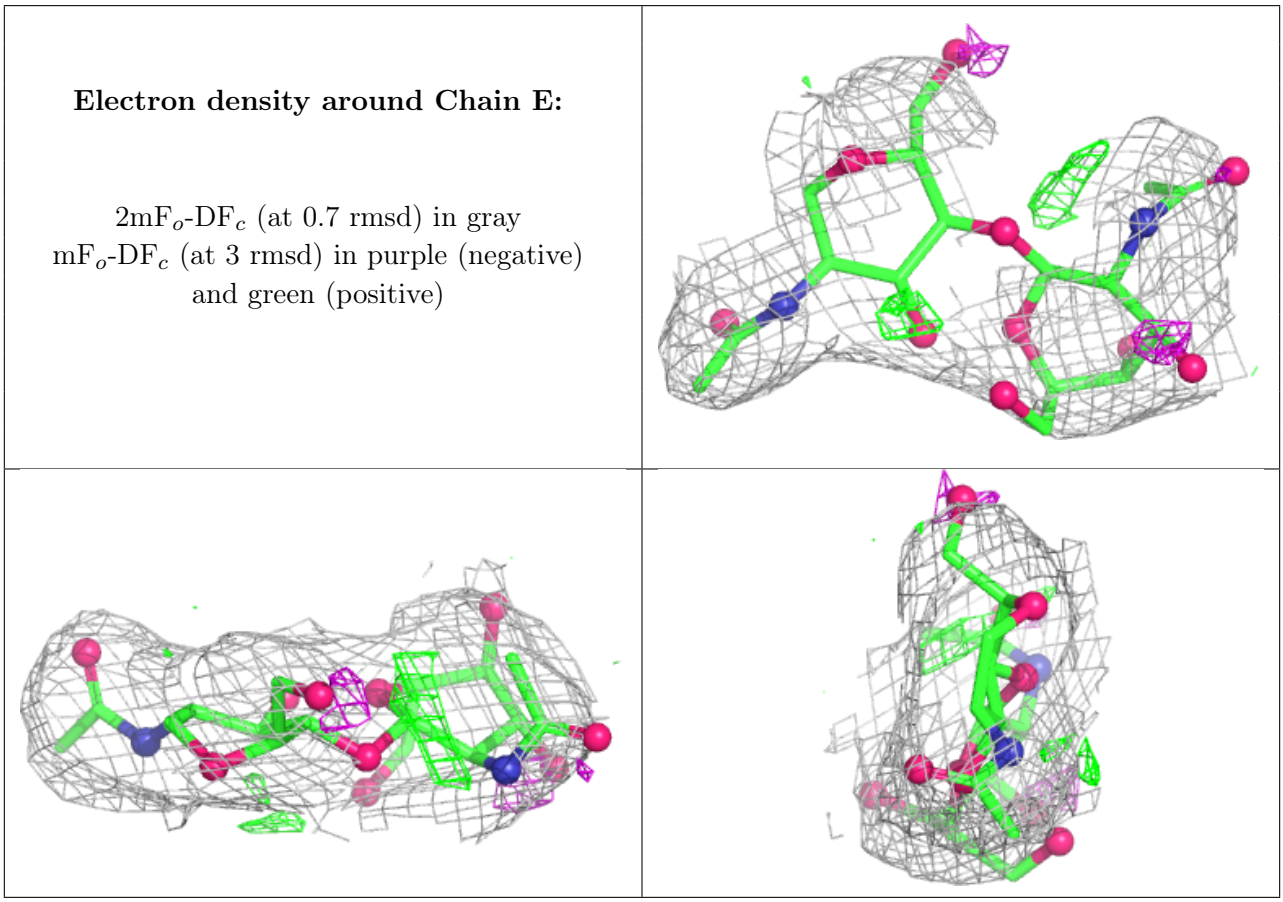
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	E	2	14/15	0.81	0.25	80,88,108,108	0
4	NAG	E	1	14/15	0.91	0.18	47,59,69,73	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	NAG	B	1001	14/15	0.56	0.27	57,60,76,82	0

6.5 Other polymers (i)

There are no such residues in this entry.