



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2020 – 05:22 PM BST

PDB ID : 6JYT
Title : Delicate structural coordination of the Severe Acute Respiratory Syndrome coronavirus Nsp13 upon ATP hydrolysis
Authors : Yan, L.; Jia, Z.
Deposited on : 2019-04-28
Resolution : 2.80 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
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) : 2.13

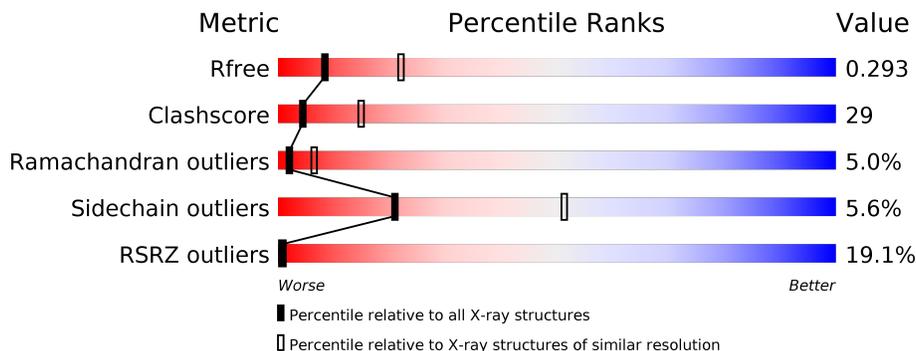
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 on 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 $\leq 5\%$. 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	603	
1	B	603	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9467 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 Helicase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	597	4655	2956	794	871	26	8	0	0	0
1	B	597	4657	2958	794	871	26	8	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ASN	-	expression tag	UNP P0C6X7
A	0	SER	-	expression tag	UNP P0C6X7
B	-1	ASN	-	expression tag	UNP P0C6X7
B	0	SER	-	expression tag	UNP P0C6X7

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Zn	0	0
			3	3		
2	A	3	Total	Zn	0	0
			3	3		

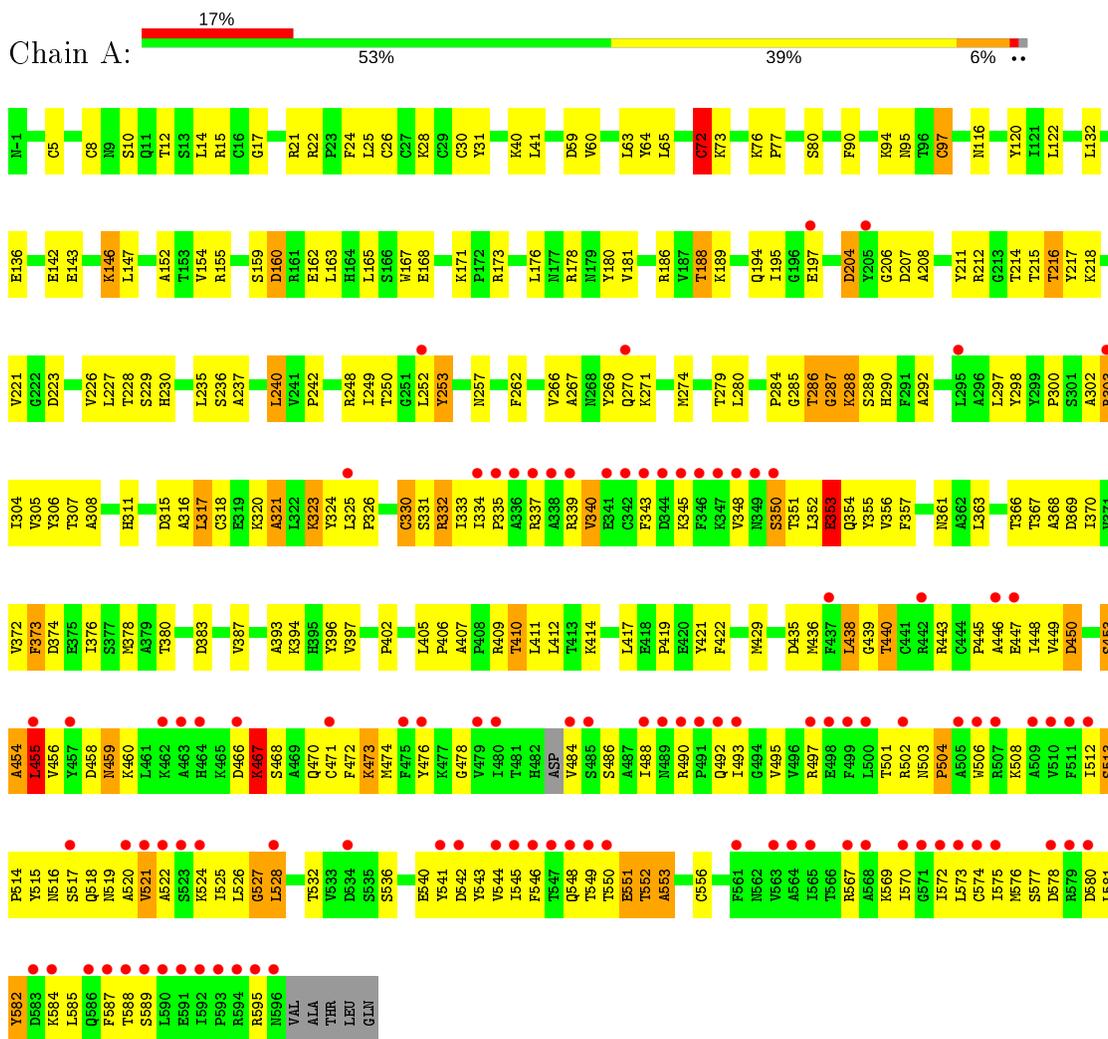
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	69	Total	O	0	0
			69	69		
3	B	80	Total	O	0	0
			80	80		

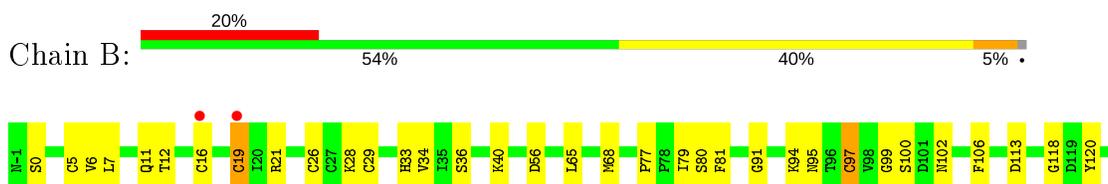
3 Residue-property plots

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: Helicase



- Molecule 1: Helicase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	191.99Å 189.15Å 57.33Å 90.00° 102.89° 90.00°	Depositor
Resolution (Å)	48.83 – 2.80 48.83 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.83-2.80) 99.4 (48.83-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.237 , 0.292 0.238 , 0.293	Depositor DCC
R_{free} test set	2533 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å ²)	57.2	Xtrriage
Anisotropy	0.909	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 73.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9467	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.52% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.64	2/4751 (0.0%)	0.80	3/6450 (0.0%)
1	B	0.68	3/4753 (0.1%)	0.81	2/6451 (0.0%)
All	All	0.66	5/9504 (0.1%)	0.80	5/12901 (0.0%)

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	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	19	CYS	CB-SG	17.20	2.11	1.82
1	A	97	CYS	CB-SG	-6.22	1.71	1.82
1	A	72	CYS	CB-SG	-5.75	1.72	1.81
1	B	19	CYS	CA-CB	5.17	1.65	1.53
1	B	97	CYS	CB-SG	-5.14	1.73	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	19	CYS	CB-CA-C	5.66	121.72	110.40
1	A	438	LEU	CA-CB-CG	5.48	127.90	115.30
1	A	221	VAL	N-CA-C	-5.39	96.44	111.00
1	A	240	LEU	CB-CG-CD2	-5.04	102.42	111.00
1	B	510	VAL	CB-CA-C	-5.03	101.85	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	353	GLU	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	4655	0	4620	263	0
1	B	4657	0	4624	272	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	69	0	0	17	0
3	B	80	0	0	25	1
All	All	9467	0	9244	534	1

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 29.

All (534) 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:19:CYS:CB	1:B:19:CYS:SG	2.11	1.37
1:B:21:ARG:NH1	1:B:136:GLU:HB3	1.43	1.34
1:B:21:ARG:HH11	1:B:136:GLU:CB	1.42	1.31
1:B:566:THR:OG1	1:B:567:ARG:NH2	1.72	1.22
1:B:21:ARG:NH1	1:B:136:GLU:OE1	1.80	1.15
1:A:334:ILE:HD11	1:A:343:PHE:O	1.47	1.13
1:B:509:ALA:C	1:B:528:LEU:HD23	1.70	1.12
1:B:447:GLU:OE1	1:B:470:GLN:NE2	1.81	1.11
1:B:427:ARG:NH1	3:B:801:HOH:O	1.81	1.11
1:B:510:VAL:HG22	1:B:511:PHE:N	1.65	1.06
1:B:510:VAL:CG2	1:B:511:PHE:N	2.18	1.06
1:A:214:THR:O	1:A:337:ARG:NH1	1.88	1.05
1:B:19:CYS:SG	1:B:33:HIS:NE2	2.30	1.01
1:B:563:VAL:HA	1:B:567:ARG:NH2	1.76	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:508:LYS:O	1:B:509:ALA:O	1.82	0.97
1:B:509:ALA:C	1:B:528:LEU:CD2	2.32	0.97
1:B:575:ILE:HD12	1:B:575:ILE:O	1.62	0.97
1:B:509:ALA:O	1:B:528:LEU:HD23	1.65	0.95
1:B:492:GLN:HG3	1:B:575:ILE:CD1	1.96	0.95
1:A:474:MSE:HE1	1:A:476:TYR:CG	2.03	0.94
1:B:285:GLY:H	1:B:288:LYS:HE3	1.31	0.93
1:A:351:THR:HG22	1:A:352:LEU:HG	1.50	0.93
1:B:21:ARG:NH1	1:B:136:GLU:CB	2.14	0.93
1:B:21:ARG:HH11	1:B:136:GLU:HB3	0.77	0.92
1:B:189:LYS:HB3	1:B:190:ASN:HB3	1.52	0.92
1:B:563:VAL:C	1:B:567:ARG:NH2	2.22	0.91
1:A:303:ARG:NH1	1:A:367:THR:O	2.04	0.90
1:A:332:ARG:HE	1:A:343:PHE:HD2	1.15	0.90
1:B:566:THR:HG1	1:B:567:ARG:NH2	1.67	0.89
1:B:455:LEU:HG	1:B:456:VAL:HG23	1.54	0.89
1:B:563:VAL:HA	1:B:567:ARG:HH22	1.37	0.88
1:A:332:ARG:NE	1:A:343:PHE:HB2	1.88	0.88
1:B:563:VAL:CA	1:B:567:ARG:NH2	2.37	0.88
1:B:330:CYS:N	1:B:353:GLU:OE1	2.08	0.87
1:A:332:ARG:NH2	1:A:343:PHE:HB2	1.89	0.87
1:B:510:VAL:CG2	1:B:511:PHE:H	1.86	0.86
1:A:474:MSE:HE1	1:A:476:TYR:CD1	2.12	0.85
1:B:566:THR:HG1	1:B:567:ARG:HH22	1.21	0.85
1:B:287:GLY:HA3	1:B:438:LEU:HD21	1.59	0.84
1:A:332:ARG:CZ	1:A:343:PHE:HB2	2.08	0.84
1:A:332:ARG:NE	1:A:343:PHE:HD2	1.75	0.84
1:B:489:ASN:H	1:B:518:GLN:HG3	1.41	0.84
1:B:330:CYS:N	3:B:808:HOH:O	2.11	0.83
1:A:168:GLU:CD	1:A:171:LYS:HE2	1.98	0.83
1:A:512:ILE:HD12	1:A:513:SER:H	1.41	0.83
1:A:21:ARG:HE	1:A:136:GLU:HG2	1.44	0.82
1:A:303:ARG:HH22	1:A:366:THR:HG21	1.45	0.82
1:B:437:PHE:HD2	1:B:438:LEU:H	1.27	0.81
1:B:189:LYS:N	1:B:190:ASN:O	2.11	0.81
1:B:492:GLN:OE1	1:B:575:ILE:HD13	1.81	0.81
1:B:510:VAL:HG23	1:B:511:PHE:H	1.45	0.81
1:A:414:LYS:NZ	3:A:803:HOH:O	2.08	0.81
1:A:332:ARG:HE	1:A:343:PHE:HB2	1.45	0.80
1:B:21:ARG:NH1	1:B:136:GLU:CG	2.45	0.79
1:A:471:CYS:HG	1:A:588:THR:HG1	1.28	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:LYS:O	1:B:290:HIS:N	2.16	0.79
1:B:21:ARG:NH1	1:B:136:GLU:CD	2.37	0.78
1:B:492:GLN:HG3	1:B:575:ILE:HD11	1.62	0.78
1:B:129:ARG:NH2	3:B:809:HOH:O	2.15	0.78
1:B:255:THR:O	3:B:802:HOH:O	2.01	0.78
1:A:262:PHE:HE1	1:A:297:LEU:HD12	1.49	0.78
1:A:311:HIS:HD1	1:A:343:PHE:HE1	1.31	0.78
1:A:332:ARG:HH21	1:A:343:PHE:HB2	1.50	0.77
1:A:286:THR:O	1:A:288:LYS:N	2.18	0.77
1:A:303:ARG:HH12	1:A:366:THR:HG22	1.47	0.77
1:B:255:THR:OG1	1:B:256:LEU:N	2.17	0.77
1:B:19:CYS:HG	1:B:33:HIS:HE2	0.84	0.77
1:A:303:ARG:HD3	1:A:303:ARG:C	2.06	0.76
1:B:159:SER:HB3	1:B:162:GLU:H	1.49	0.76
1:A:332:ARG:NE	1:A:343:PHE:CD2	2.53	0.76
1:A:248:ARG:NH1	1:A:249:ILE:O	2.19	0.75
1:A:512:ILE:HD12	1:A:513:SER:N	2.02	0.74
1:A:450:ASP:HA	1:A:453:SER:HB3	1.70	0.74
1:A:526:LEU:HD22	1:A:528:LEU:HD11	1.69	0.74
1:A:94:LYS:O	3:A:801:HOH:O	2.05	0.74
1:A:320:LYS:HA	1:A:323:LYS:HE2	1.70	0.73
1:B:287:GLY:CA	1:B:438:LEU:HD21	2.19	0.73
1:A:181:VAL:O	3:A:802:HOH:O	2.08	0.72
1:A:334:ILE:CD1	1:A:343:PHE:O	2.34	0.72
1:B:186:ARG:NH1	3:B:815:HOH:O	2.22	0.71
1:B:563:VAL:C	1:B:567:ARG:CZ	2.59	0.71
1:B:68:MSE:HG2	3:B:823:HOH:O	1.89	0.71
1:A:473:LYS:HB3	1:A:589:SER:HA	1.71	0.71
1:B:510:VAL:N	1:B:528:LEU:HD22	2.06	0.70
1:A:188:THR:OG1	1:A:189:LYS:N	2.24	0.70
1:B:286:THR:H	1:B:288:LYS:HD2	1.56	0.70
1:A:376:ILE:HD11	1:A:429:MSE:HE2	1.74	0.70
1:B:564:ALA:CA	1:B:567:ARG:HE	2.05	0.70
1:A:266:VAL:HG22	1:A:298:TYR:HE1	1.55	0.70
1:B:488:ILE:HA	1:B:518:GLN:HB2	1.73	0.70
1:B:474:MSE:SE	1:B:582:TYR:HB3	2.41	0.70
1:A:267:ALA:C	1:A:270:GLN:HG3	2.11	0.69
1:A:147:LEU:O	3:A:804:HOH:O	2.09	0.69
1:B:305:VAL:HG22	1:B:371:VAL:HG22	1.73	0.69
1:A:320:LYS:NZ	3:A:812:HOH:O	2.23	0.69
1:A:303:ARG:HH12	1:A:366:THR:CG2	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:CYS:HA	1:B:587:PHE:HB3	1.72	0.69
1:B:297:LEU:N	3:B:813:HOH:O	2.25	0.69
1:B:28:LYS:HG3	1:B:97:CYS:SG	2.33	0.68
1:B:548:GLN:HG3	1:B:576:MSE:HB2	1.75	0.68
1:A:162:GLU:O	1:A:163:LEU:HD23	1.92	0.68
1:B:36:SER:OG	3:B:805:HOH:O	2.10	0.68
1:B:564:ALA:C	1:B:567:ARG:HE	1.96	0.68
1:B:179:ASN:N	3:B:811:HOH:O	2.18	0.68
1:B:449:VAL:HG11	1:B:463:ALA:HB2	1.75	0.68
1:B:21:ARG:HH12	1:B:136:GLU:CD	1.98	0.67
1:B:262:PHE:HE2	1:B:297:LEU:HD12	1.59	0.67
1:A:513:SER:OG	1:A:519:ASN:OD1	2.11	0.67
1:B:250:THR:N	3:B:817:HOH:O	2.27	0.67
1:B:355:TYR:OH	3:B:806:HOH:O	2.10	0.67
1:A:330:CYS:HB2	1:A:355:TYR:HB2	1.77	0.67
1:B:576:MSE:HG2	1:B:577:SER:N	2.09	0.67
1:B:242:PRO:O	3:B:807:HOH:O	2.11	0.67
1:B:564:ALA:N	1:B:567:ARG:HH21	1.93	0.67
1:A:459:ASN:C	1:A:460:LYS:HD3	2.16	0.66
1:A:40:LYS:HD2	1:A:59:ASP:OD1	1.96	0.66
1:A:446:ALA:HB3	1:A:467:LYS:HD2	1.76	0.66
1:B:152:ALA:HB2	1:B:167:TRP:CZ3	2.32	0.65
1:A:332:ARG:HE	1:A:343:PHE:CB	2.09	0.65
1:A:354:GLN:HG2	1:A:355:TYR:CE2	2.31	0.65
1:A:549:THR:O	1:A:577:SER:OG	2.07	0.65
1:A:142:GLU:HG2	1:A:411:LEU:HD12	1.78	0.65
1:A:574:CYS:HB3	1:A:576:MSE:HE2	1.79	0.65
1:A:333:ILE:HG13	1:A:334:ILE:H	1.62	0.65
1:A:497:ARG:O	1:A:501:THR:OG1	2.15	0.65
1:A:333:ILE:O	1:A:334:ILE:HD13	1.98	0.64
1:A:471:CYS:SG	1:A:588:THR:OG1	2.52	0.64
1:B:289:SER:O	1:B:293:ILE:HG12	1.98	0.64
1:A:303:ARG:HD2	1:A:368:ALA:HA	1.80	0.64
1:A:12:THR:HB	1:A:26:CYS:HA	1.79	0.64
1:A:207:ASP:OD2	3:A:805:HOH:O	2.15	0.64
1:A:526:LEU:HD22	1:A:528:LEU:CD1	2.28	0.64
1:B:472:PHE:HD1	1:B:587:PHE:HB2	1.63	0.64
1:A:514:PRO:HD3	1:A:546:PHE:HE2	1.63	0.64
1:B:269:TYR:CD2	1:B:295:LEU:HD13	2.33	0.63
1:A:582:TYR:HA	1:A:585:LEU:HG	1.79	0.63
1:A:21:ARG:NE	1:A:136:GLU:HG2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:ALA:O	1:A:306:TYR:OH	2.08	0.63
1:A:280:LEU:HD11	1:A:438:LEU:HD23	1.80	0.63
1:A:372:VAL:HG13	1:A:397:VAL:HG13	1.80	0.62
1:A:77:PRO:HG2	1:A:80:SER:HB3	1.81	0.62
1:A:473:LYS:NZ	1:A:578:ASP:OD2	2.26	0.62
1:B:472:PHE:CD1	1:B:587:PHE:HB2	2.34	0.62
1:B:332:ARG:HD2	1:B:347:LYS:O	2.00	0.62
1:B:472:PHE:HD2	1:B:474:MSE:HG3	1.65	0.62
1:B:284:PRO:HG2	1:B:566:THR:HG21	1.80	0.62
1:A:306:TYR:CD1	1:A:317:LEU:HD21	2.35	0.61
1:A:545:ILE:HG23	1:A:573:LEU:HG	1.81	0.61
1:B:322:LEU:HD22	1:B:327:ILE:HD12	1.82	0.61
1:A:159:SER:HB3	1:A:162:GLU:H	1.65	0.61
1:A:542:ASP:HB3	1:A:570:ILE:HD12	1.82	0.61
1:B:547:THR:HG23	1:B:575:ILE:HD11	1.81	0.61
1:B:332:ARG:HH22	1:B:345:LYS:HB2	1.65	0.61
1:B:218:LYS:O	3:B:810:HOH:O	2.16	0.61
1:B:427:ARG:NE	3:B:814:HOH:O	2.21	0.61
1:A:553:ALA:HA	1:A:556:CYS:HB3	1.83	0.61
1:B:21:ARG:HH12	1:B:136:GLU:CG	2.13	0.61
1:A:402:PRO:HG3	1:A:429:MSE:HE3	1.83	0.61
1:A:443:ARG:NH2	1:A:567:ARG:HA	2.16	0.60
1:B:302:ALA:O	1:B:304:ILE:HG13	2.01	0.60
1:B:286:THR:OG1	1:B:287:GLY:N	2.33	0.60
1:B:297:LEU:O	1:B:300:PRO:HG3	2.00	0.60
1:A:576:MSE:HE3	1:A:585:LEU:HD22	1.83	0.60
1:B:269:TYR:HD2	1:B:295:LEU:HD13	1.66	0.60
1:B:509:ALA:O	1:B:528:LEU:CD2	2.45	0.60
1:A:22:ARG:NH2	1:B:56:ASP:O	2.32	0.60
1:B:21:ARG:CZ	1:B:136:GLU:OE1	2.49	0.60
1:B:532:THR:O	1:B:536:SER:OG	2.18	0.60
1:B:177:ASN:HB3	3:B:811:HOH:O	2.01	0.59
1:A:287:GLY:N	3:A:817:HOH:O	2.35	0.59
1:B:304:ILE:HG12	1:B:370:ILE:HG23	1.84	0.59
1:B:143:GLU:HG3	1:B:230:HIS:O	2.01	0.59
1:A:214:THR:OG1	1:A:337:ARG:HD3	2.02	0.59
1:A:373:PHE:CE2	1:A:387:VAL:HG21	2.38	0.59
1:A:473:LYS:HG3	1:A:474:MSE:N	2.17	0.59
1:B:549:THR:OG1	1:B:550:THR:N	2.35	0.59
1:B:566:THR:OG1	1:B:567:ARG:CZ	2.48	0.59
1:B:266:VAL:O	1:B:270:GLN:HG3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:PRO:HG3	1:B:570:ILE:HA	1.83	0.59
1:B:585:LEU:HB2	1:B:587:PHE:HE2	1.67	0.58
1:A:473:LYS:HG3	1:A:474:MSE:H	1.67	0.58
1:A:497:ARG:HD2	1:A:525:ILE:HD11	1.85	0.58
1:A:454:ALA:O	1:A:456:VAL:N	2.32	0.58
1:A:60:VAL:HA	1:A:63:LEU:HD12	1.86	0.58
1:B:484:VAL:HG23	1:B:486:SER:H	1.67	0.58
1:A:303:ARG:HD3	1:A:304:ILE:N	2.18	0.58
1:A:471:CYS:HB2	1:A:587:PHE:HB3	1.84	0.58
1:A:242:PRO:O	3:A:807:HOH:O	2.17	0.58
1:A:332:ARG:CD	1:A:343:PHE:HD2	2.17	0.57
1:B:564:ALA:N	1:B:567:ARG:NH2	2.52	0.57
1:A:526:LEU:HD22	1:A:528:LEU:CG	2.33	0.57
1:B:271:LYS:O	1:B:274:MSE:N	2.24	0.57
1:A:472:PHE:CE1	1:A:572:ILE:HG23	2.39	0.57
1:B:187:VAL:HG22	1:B:192:LYS:HD3	1.87	0.57
1:B:34:VAL:O	1:B:40:LYS:HE3	2.04	0.57
1:B:509:ALA:C	1:B:528:LEU:HD22	2.21	0.57
1:A:311:HIS:CD2	1:A:339:ARG:HG2	2.40	0.57
1:A:64:TYR:CD1	1:A:76:LYS:HD3	2.39	0.57
1:B:348:VAL:HG23	1:B:349:ASN:H	1.70	0.57
1:A:186:ARG:NH1	1:A:217:TYR:OH	2.37	0.57
1:B:334:ILE:HB	1:B:343:PHE:HE2	1.70	0.57
1:B:548:GLN:CG	1:B:576:MSE:HB2	2.34	0.57
1:A:155:ARG:NH2	3:A:820:HOH:O	2.37	0.57
1:B:575:ILE:CD1	1:B:575:ILE:O	2.46	0.57
1:B:563:VAL:O	1:B:567:ARG:CZ	2.52	0.57
1:B:259:SER:HB2	1:B:261:GLU:OE1	2.05	0.56
1:B:77:PRO:HG2	1:B:80:SER:HB3	1.87	0.56
1:A:334:ILE:HD11	1:A:343:PHE:C	2.25	0.56
1:B:477:LYS:HA	1:B:492:GLN:NE2	2.19	0.56
1:B:447:GLU:CD	1:B:470:GLN:NE2	2.58	0.56
1:A:17:GLY:HA3	1:A:41:LEU:HD23	1.88	0.56
1:A:361:ASN:N	3:A:816:HOH:O	2.35	0.56
1:A:455:LEU:HD22	1:A:584:LYS:HE2	1.88	0.56
1:B:492:GLN:CG	1:B:575:ILE:CD1	2.77	0.56
1:B:490:ARG:HA	1:B:493:ILE:HG12	1.88	0.56
1:B:303:ARG:HG3	1:B:368:ALA:HA	1.88	0.56
1:A:311:HIS:ND1	1:A:343:PHE:HE1	2.02	0.56
1:A:419:PRO:HA	1:A:422:PHE:CE2	2.41	0.56
1:B:279:THR:HB	1:B:429:MSE:HE2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:486:SER:HB3	1:B:515:TYR:HB3	1.87	0.55
1:A:154:VAL:HG23	1:A:223:ASP:O	2.06	0.55
1:B:177:ASN:HB3	1:B:180:TYR:HD2	1.71	0.55
1:A:307:THR:HG21	1:A:363:LEU:HD11	1.88	0.55
1:B:315:ASP:O	1:B:318:CYS:N	2.31	0.55
1:A:472:PHE:CD1	1:A:573:LEU:HA	2.42	0.55
1:B:533:VAL:HG23	1:B:534:ASP:OD1	2.07	0.55
1:A:214:THR:HB	1:A:337:ARG:HH11	1.72	0.55
1:B:557:ASN:HB3	1:B:560:ARG:HB2	1.88	0.54
1:B:406:PRO:HB3	1:B:422:PHE:CZ	2.43	0.54
1:A:267:ALA:HA	1:A:270:GLN:HG3	1.90	0.54
1:B:437:PHE:HD2	1:B:438:LEU:N	2.02	0.54
1:B:545:ILE:HG23	1:B:573:LEU:HG	1.90	0.54
1:A:197:GLU:OE2	1:A:337:ARG:HG2	2.08	0.54
1:B:197:GLU:H	1:B:214:THR:HB	1.73	0.54
1:B:118:GLY:N	3:B:818:HOH:O	2.30	0.54
1:B:126:CYS:SG	1:B:130:LEU:HB3	2.47	0.54
1:B:254:PRO:HB3	1:B:298:TYR:CE1	2.43	0.54
1:A:303:ARG:NH2	1:A:366:THR:HG21	2.19	0.53
1:A:474:MSE:CE	1:A:476:TYR:CD1	2.88	0.53
1:A:267:ALA:O	1:A:270:GLN:HG3	2.09	0.53
1:B:5:CYS:HB2	1:B:26:CYS:HB3	1.90	0.53
1:A:284:PRO:HB3	1:A:567:ARG:HH12	1.73	0.53
1:A:331:SER:HA	1:A:345:LYS:HG3	1.90	0.53
1:A:515:TYR:CE2	1:A:549:THR:HG21	2.44	0.53
1:B:518:GLN:HA	1:B:521:VAL:HG22	1.90	0.53
1:A:332:ARG:CD	1:A:343:PHE:CD2	2.92	0.53
1:A:354:GLN:HG2	1:A:355:TYR:CZ	2.43	0.53
1:B:241:VAL:HG22	1:B:242:PRO:HD2	1.89	0.53
1:B:509:ALA:CA	1:B:528:LEU:HD23	2.38	0.53
1:A:214:THR:C	1:A:337:ARG:NH1	2.60	0.53
1:B:477:LYS:HD3	1:B:492:GLN:NE2	2.23	0.53
1:A:143:GLU:HG3	1:A:230:HIS:O	2.09	0.53
1:A:472:PHE:HE1	1:A:572:ILE:HG23	1.72	0.53
1:A:526:LEU:HD13	1:A:528:LEU:HD11	1.91	0.53
1:A:323:LYS:O	1:A:325:LEU:N	2.42	0.52
1:A:473:LYS:HE2	1:A:582:TYR:HD1	1.74	0.52
1:B:473:LYS:HD2	1:B:590:LEU:HB3	1.91	0.52
1:A:460:LYS:HD3	1:A:460:LYS:N	2.25	0.52
1:B:239:THR:O	1:B:388:ASN:ND2	2.42	0.52
1:A:267:ALA:CA	1:A:270:GLN:HG3	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:PHE:HE1	1:B:290:HIS:NE2	2.07	0.52
1:B:576:MSE:HG2	1:B:577:SER:H	1.74	0.52
1:A:132:LEU:HD21	1:A:237:ALA:O	2.09	0.52
1:A:286:THR:HG23	1:A:289:SER:H	1.75	0.52
1:A:332:ARG:NE	1:A:343:PHE:CB	2.66	0.52
1:A:578:ASP:OD1	1:A:581:LEU:N	2.42	0.52
1:B:582:TYR:HA	1:B:585:LEU:HG	1.91	0.52
1:B:254:PRO:HB3	1:B:298:TYR:HE1	1.75	0.52
1:A:445:PRO:O	1:A:449:VAL:HG23	2.10	0.51
1:B:286:THR:N	1:B:288:LYS:HD2	2.24	0.51
1:B:333:ILE:HG22	1:B:334:ILE:HG12	1.93	0.51
1:A:369:ASP:O	1:A:370:ILE:HD13	2.11	0.51
1:B:287:GLY:N	1:B:438:LEU:HD21	2.26	0.51
1:B:488:ILE:HD11	1:B:517:SER:HB2	1.93	0.51
1:B:477:LYS:HA	1:B:492:GLN:HE22	1.75	0.51
1:B:68:MSE:N	3:B:823:HOH:O	2.33	0.51
1:B:471:CYS:SG	3:B:875:HOH:O	2.59	0.50
1:A:473:LYS:HZ3	1:A:582:TYR:HB3	1.75	0.50
1:B:489:ASN:CG	1:B:492:GLN:HB2	2.32	0.50
1:A:297:LEU:O	1:A:300:PRO:HG3	2.12	0.50
1:A:380:THR:O	1:A:383:ASP:N	2.41	0.50
1:B:292:ALA:O	1:B:306:TYR:OH	2.23	0.50
1:B:515:TYR:CD2	1:B:549:THR:HG21	2.47	0.50
1:A:549:THR:HG23	1:A:551:GLU:H	1.77	0.50
1:B:564:ALA:HA	1:B:567:ARG:HE	1.76	0.50
1:A:72:CYS:O	1:A:76:LYS:HB2	2.12	0.50
1:B:286:THR:HB	1:B:441:CYS:HA	1.92	0.50
1:B:477:LYS:HD3	1:B:492:GLN:HE21	1.77	0.49
1:A:317:LEU:HD23	1:A:357:PHE:HE2	1.78	0.49
1:A:393:ALA:C	1:A:394:LYS:HE2	2.33	0.49
1:B:385:SER:OG	3:B:812:HOH:O	2.20	0.49
1:A:228:THR:OG1	3:A:809:HOH:O	2.20	0.49
1:A:250:THR:O	3:A:808:HOH:O	2.19	0.49
1:A:90:PHE:CD1	1:A:94:LYS:HE3	2.48	0.49
1:B:473:LYS:O	1:B:475:PHE:N	2.46	0.49
1:A:21:ARG:HE	1:A:136:GLU:CG	2.18	0.49
1:A:8:CYS:SG	1:A:10:SER:OG	2.60	0.49
1:B:127:THR:HG22	1:B:129:ARG:H	1.78	0.49
1:A:473:LYS:HD2	1:A:585:LEU:HD11	1.94	0.49
1:B:437:PHE:CD2	1:B:438:LEU:N	2.78	0.49
1:A:308:ALA:HB2	1:A:374:ASP:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:580:ASP:O	1:B:584:LYS:HD2	2.12	0.49
1:B:262:PHE:CE2	1:B:297:LEU:HD12	2.44	0.49
1:A:473:LYS:NZ	1:A:582:TYR:HB3	2.28	0.48
1:B:566:THR:H	1:B:567:ARG:NH2	2.11	0.48
1:A:271:LYS:O	1:A:274:MSE:N	2.47	0.48
1:A:303:ARG:NH1	1:A:366:THR:HG22	2.22	0.48
1:A:526:LEU:HD22	1:A:528:LEU:HG	1.95	0.48
1:A:532:THR:O	1:A:536:SER:OG	2.27	0.48
1:B:445:PRO:O	1:B:449:VAL:HG23	2.12	0.48
1:A:152:ALA:HB2	1:A:167:TRP:CZ3	2.47	0.48
1:A:194:GLN:HG3	1:A:195:ILE:N	2.28	0.48
1:A:406:PRO:HB3	1:A:422:PHE:CZ	2.48	0.48
1:B:478:GLY:H	1:B:492:GLN:NE2	2.12	0.48
1:A:417:LEU:HD22	1:A:421:TYR:HB2	1.96	0.48
1:A:168:GLU:OE1	1:A:171:LYS:HE2	2.13	0.48
1:A:214:THR:CB	1:A:337:ARG:HH11	2.24	0.48
1:B:143:GLU:O	1:B:229:SER:HB2	2.14	0.48
1:B:380:THR:O	1:B:383:ASP:N	2.43	0.48
1:B:492:GLN:HG3	1:B:575:ILE:HD13	1.87	0.48
1:A:214:THR:CB	1:A:337:ARG:HD3	2.44	0.48
1:B:280:LEU:HB3	1:B:399:ILE:HG23	1.96	0.47
1:A:159:SER:O	1:A:218:LYS:NZ	2.44	0.47
1:A:353:GLU:HG3	1:A:354:GLN:N	2.29	0.47
1:B:508:LYS:O	1:B:509:ALA:C	2.50	0.47
1:A:361:ASN:HB2	3:A:816:HOH:O	2.13	0.47
1:A:443:ARG:HH21	1:A:567:ARG:HA	1.79	0.47
1:A:73:LYS:HA	1:A:76:LYS:HE2	1.97	0.47
1:B:581:LEU:HG	1:B:585:LEU:HD23	1.96	0.47
1:A:214:THR:HB	1:A:337:ARG:NH1	2.29	0.47
1:A:540:GLU:HB3	1:A:569:LYS:HE3	1.96	0.47
1:A:163:LEU:HG	1:A:211:TYR:CD1	2.49	0.47
1:B:266:VAL:HG13	1:B:298:TYR:CE2	2.50	0.47
1:B:545:ILE:HD12	1:B:573:LEU:HD21	1.96	0.47
1:A:317:LEU:HD23	1:A:357:PHE:CE2	2.50	0.47
1:A:376:ILE:HD11	1:A:429:MSE:CE	2.44	0.47
1:A:490:ARG:HA	1:A:493:ILE:HG12	1.96	0.47
1:A:544:VAL:HG13	1:A:572:ILE:HD13	1.97	0.47
1:B:559:ASN:ND2	3:B:828:HOH:O	2.47	0.47
1:A:581:LEU:HG	1:A:585:LEU:HD23	1.97	0.47
1:B:334:ILE:CG2	1:B:337:ARG:H	2.28	0.47
1:A:262:PHE:CE1	1:A:297:LEU:HD12	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:ILE:HG13	1:A:517:SER:HB2	1.97	0.46
1:A:521:VAL:HG12	1:A:524:LYS:HE2	1.97	0.46
1:B:227:LEU:HD12	1:B:227:LEU:HA	1.53	0.46
1:A:378:MSE:HB3	1:A:378:MSE:HE3	1.79	0.46
1:A:446:ALA:HA	1:A:449:VAL:HB	1.97	0.46
1:B:246:TYR:HB2	1:B:274:MSE:HA	1.96	0.46
1:B:256:LEU:HB3	1:B:257:ASN:H	1.49	0.46
1:B:458:ASP:N	3:B:829:HOH:O	2.48	0.46
1:B:576:MSE:SE	1:B:578:ASP:HB2	2.65	0.46
1:B:585:LEU:HB2	1:B:587:PHE:CE2	2.49	0.46
1:B:163:LEU:O	1:B:208:ALA:HA	2.16	0.46
1:B:267:ALA:O	1:B:270:GLN:HB2	2.15	0.46
1:B:563:VAL:O	1:B:563:VAL:HG12	2.15	0.46
1:B:428:LEU:HA	1:B:428:LEU:HD23	1.69	0.46
1:B:79:ILE:HD12	1:B:79:ILE:HA	1.82	0.46
1:A:551:GLU:HA	1:A:552:THR:O	2.16	0.46
1:B:457:TYR:HB3	3:B:829:HOH:O	2.15	0.46
1:A:393:ALA:HB3	1:A:396:TYR:CZ	2.50	0.46
1:A:466:ASP:O	1:A:468:SER:N	2.35	0.46
1:A:5:CYS:HB2	1:A:26:CYS:HB3	1.97	0.46
1:A:64:TYR:CG	1:A:76:LYS:HD3	2.51	0.46
1:B:139:LYS:HD3	1:B:232:VAL:HG13	1.98	0.46
1:B:477:LYS:NZ	1:B:576:MSE:HA	2.31	0.46
1:B:311:HIS:O	1:B:314:VAL:HG12	2.16	0.45
1:B:515:TYR:HD2	1:B:549:THR:HG21	1.81	0.45
1:B:142:GLU:HG2	1:B:411:LEU:HD12	1.98	0.45
1:A:321:ALA:O	1:A:325:LEU:HB2	2.17	0.45
1:B:544:VAL:HG13	1:B:572:ILE:HD13	1.98	0.45
1:A:215:THR:O	1:A:216:THR:HG22	2.15	0.45
1:A:439:GLY:HA2	1:A:440:THR:HB	1.98	0.45
1:A:503:ASN:OD1	1:A:504:PRO:HD2	2.17	0.45
1:A:473:LYS:NZ	1:A:585:LEU:HD21	2.32	0.45
1:B:334:ILE:HG13	1:B:338:ALA:HB2	1.97	0.45
1:B:513:SER:HA	1:B:546:PHE:HE2	1.81	0.45
1:A:515:TYR:HE2	1:A:549:THR:HG21	1.81	0.45
1:A:146:LYS:HG2	1:A:146:LYS:HZ2	1.63	0.45
1:B:276:LYS:HD2	1:B:276:LYS:O	2.17	0.45
1:B:315:ASP:O	1:B:317:LEU:N	2.50	0.45
1:B:398:TYR:OH	3:B:803:HOH:O	2.04	0.45
1:B:541:TYR:O	1:B:569:LYS:HG3	2.17	0.45
1:A:218:LYS:N	3:A:829:HOH:O	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:THR:O	1:A:435:ASP:HB2	2.17	0.45
1:B:484:VAL:HG23	1:B:486:SER:N	2.31	0.45
1:B:510:VAL:HG23	1:B:511:PHE:N	2.07	0.45
1:B:448:ILE:HD13	1:B:565:ILE:HG22	1.99	0.45
1:A:214:THR:C	1:A:337:ARG:HH11	2.20	0.45
1:A:122:LEU:HD12	1:A:122:LEU:HA	1.68	0.45
1:A:15:ARG:HD2	1:A:24:PHE:CE1	2.52	0.45
1:B:94:LYS:HB2	1:B:94:LYS:HE3	1.74	0.45
1:A:285:GLY:N	1:A:286:THR:HA	2.32	0.44
1:B:157:VAL:HA	1:B:163:LEU:HD12	1.99	0.44
1:B:325:LEU:HD22	1:B:355:TYR:CE2	2.52	0.44
1:A:303:ARG:CD	1:A:303:ARG:C	2.82	0.44
1:B:261:GLU:N	1:B:261:GLU:OE1	2.32	0.44
1:A:478:GLY:H	1:A:492:GLN:NE2	2.15	0.44
1:A:514:PRO:HD3	1:A:546:PHE:CE2	2.48	0.44
1:A:541:TYR:O	1:A:569:LYS:N	2.51	0.44
1:B:453:SER:HB3	1:B:459:ASN:HA	1.99	0.44
1:A:315:ASP:O	1:A:317:LEU:N	2.51	0.44
1:A:315:ASP:O	1:A:318:CYS:N	2.30	0.44
1:B:490:ARG:N	1:B:491:PRO:HD2	2.33	0.44
1:B:154:VAL:HG23	1:B:223:ASP:O	2.18	0.44
1:B:269:TYR:O	1:B:299:TYR:OH	2.27	0.44
1:A:506:TRP:HZ3	1:A:570:ILE:HD13	1.83	0.44
1:B:489:ASN:OD1	1:B:492:GLN:HB2	2.18	0.44
1:A:333:ILE:C	1:A:334:ILE:HD13	2.37	0.44
1:A:447:GLU:HG3	1:A:448:ILE:HG23	2.00	0.44
1:B:323:LYS:N	1:B:323:LYS:HD2	2.33	0.44
1:A:226:VAL:HG23	1:A:228:THR:HG23	1.99	0.43
1:B:440:THR:HG23	1:B:463:ALA:HA	2.00	0.43
1:B:511:PHE:HE2	1:B:519:ASN:HA	1.82	0.43
1:B:315:ASP:C	1:B:317:LEU:H	2.21	0.43
1:B:550:THR:C	1:B:552:THR:H	2.21	0.43
1:B:65:LEU:HD23	1:B:81:PHE:CZ	2.52	0.43
1:A:350:SER:HA	1:A:351:THR:HA	1.53	0.43
1:A:448:ILE:HG21	1:A:572:ILE:HG21	2.00	0.43
1:B:159:SER:HB3	1:B:162:GLU:N	2.27	0.43
1:B:332:ARG:HG3	1:B:347:LYS:HE2	2.01	0.43
1:B:120:TYR:CE2	1:B:412:LEU:HB2	2.54	0.43
1:A:146:LYS:HE3	3:A:858:HOH:O	2.19	0.43
1:A:549:THR:OG1	1:A:550:THR:N	2.50	0.43
1:B:267:ALA:HA	1:B:270:GLN:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:LEU:HD23	1:A:176:LEU:HA	1.79	0.43
1:A:270:GLN:O	1:A:274:MSE:HG2	2.18	0.43
1:A:286:THR:C	1:A:288:LYS:N	2.72	0.43
1:A:417:LEU:HD23	1:A:417:LEU:HA	1.77	0.43
1:B:394:LYS:HE2	1:B:394:LYS:N	2.34	0.43
1:B:401:ASP:OD2	1:B:404:GLN:HG3	2.19	0.43
1:A:215:THR:O	1:A:217:TYR:N	2.50	0.43
1:B:510:VAL:CA	1:B:528:LEU:HD22	2.48	0.43
1:B:6:VAL:HG13	1:B:7:LEU:HG	1.99	0.43
1:A:178:ARG:O	1:A:178:ARG:HG3	2.18	0.43
1:B:315:ASP:C	1:B:317:LEU:N	2.71	0.43
1:B:412:LEU:HD12	1:B:414:LYS:H	1.83	0.42
1:B:578:ASP:OD1	1:B:581:LEU:N	2.33	0.42
1:A:120:TYR:CE2	1:A:412:LEU:HG	2.55	0.42
1:A:512:ILE:O	1:A:519:ASN:OD1	2.38	0.42
1:B:287:GLY:H	1:B:438:LEU:HD21	1.84	0.42
1:B:12:THR:HB	1:B:26:CYS:HA	2.01	0.42
1:B:186:ARG:NH1	1:B:220:ASN:OD1	2.53	0.42
1:B:248:ARG:HH21	1:B:250:THR:HA	1.84	0.42
1:B:413:THR:OG1	1:B:413:THR:O	2.36	0.42
1:B:417:LEU:HD23	1:B:417:LEU:HA	1.69	0.42
1:A:240:LEU:HA	1:A:240:LEU:HD23	1.64	0.42
1:A:262:PHE:HE2	1:A:290:HIS:NE2	2.17	0.42
1:A:567:ARG:N	1:A:567:ARG:HD2	2.34	0.42
1:B:564:ALA:CA	1:B:567:ARG:NE	2.79	0.42
1:B:29:CYS:SG	1:B:99:GLY:HA2	2.59	0.42
1:A:292:ALA:HB1	1:A:306:TYR:HE1	1.85	0.42
1:A:305:VAL:HG22	1:A:356:VAL:HB	2.01	0.42
1:A:503:ASN:HA	1:A:504:PRO:HD2	1.83	0.42
1:A:520:ALA:C	1:A:522:ALA:H	2.22	0.42
1:B:250:THR:C	1:B:252:LEU:H	2.21	0.42
1:B:585:LEU:HD12	1:B:585:LEU:O	2.19	0.42
1:A:28:LYS:HG3	1:A:97:CYS:SG	2.60	0.42
1:A:248:ARG:NH1	1:A:249:ILE:C	2.73	0.42
1:A:525:ILE:O	1:A:527:GLY:N	2.46	0.42
1:A:572:ILE:HD12	1:A:573:LEU:H	1.84	0.42
1:B:284:PRO:HG2	1:B:566:THR:CG2	2.49	0.42
1:B:410:THR:HG22	1:B:411:LEU:N	2.34	0.42
1:A:518:GLN:HA	1:A:521:VAL:HG22	2.01	0.42
1:A:76:LYS:HB3	1:A:76:LYS:HE3	1.71	0.42
1:B:176:LEU:N	1:B:176:LEU:HD22	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:VAL:HG23	1:B:530:THR:HA	2.02	0.42
1:A:168:GLU:OE2	1:A:171:LYS:HE2	2.19	0.42
1:A:252:LEU:HD12	1:A:253:TYR:CE1	2.54	0.42
1:B:335:PRO:HG2	1:B:337:ARG:HH11	1.84	0.42
1:B:474:MSE:CE	1:B:585:LEU:HD21	2.50	0.42
1:B:118:GLY:CA	3:B:818:HOH:O	2.68	0.42
1:B:541:TYR:HD1	1:B:567:ARG:HB3	1.85	0.42
1:A:302:ALA:O	1:A:304:ILE:HG13	2.20	0.41
1:A:31:TYR:C	1:A:31:TYR:CD2	2.93	0.41
1:A:409:ARG:O	1:A:410:THR:C	2.58	0.41
1:A:472:PHE:CG	1:A:573:LEU:HA	2.55	0.41
1:B:474:MSE:HE1	1:B:582:TYR:HB3	2.01	0.41
1:A:235:LEU:HD23	1:A:235:LEU:HA	1.73	0.41
1:A:250:THR:N	3:A:808:HOH:O	2.53	0.41
1:A:25:LEU:HD13	1:A:30:CYS:HA	2.02	0.41
1:A:405:LEU:HA	1:A:406:PRO:HD3	1.88	0.41
1:B:16:CYS:CB	1:B:19:CYS:SG	3.08	0.41
1:B:307:THR:HG22	1:B:372:VAL:O	2.20	0.41
1:B:419:PRO:HA	1:B:422:PHE:CE2	2.54	0.41
1:B:7:LEU:HD21	1:B:106:PHE:HB2	2.01	0.41
1:B:113:ASP:OD1	1:B:113:ASP:C	2.58	0.41
1:B:294:GLY:C	3:B:813:HOH:O	2.57	0.41
1:A:495:VAL:HG22	1:A:495:VAL:O	2.20	0.41
1:A:515:TYR:OH	1:A:549:THR:HG21	2.21	0.41
1:B:318:CYS:O	1:B:322:LEU:HG	2.21	0.41
1:B:541:TYR:CD1	1:B:567:ARG:HB3	2.55	0.41
1:A:14:LEU:HD21	1:A:90:PHE:O	2.20	0.41
1:A:315:ASP:C	1:A:317:LEU:N	2.73	0.41
1:A:325:LEU:HA	1:A:326:PRO:HD3	1.81	0.41
1:A:476:TYR:HE1	1:A:595:ARG:HH12	1.66	0.41
1:A:484:VAL:HG23	1:A:486:SER:H	1.84	0.41
1:A:65:LEU:HD12	1:A:65:LEU:HA	1.82	0.41
1:B:330:CYS:SG	1:B:331:SER:N	2.91	0.41
1:B:450:ASP:HA	1:B:453:SER:OG	2.21	0.41
1:B:457:TYR:C	1:B:459:ASN:H	2.24	0.41
1:B:492:GLN:CG	1:B:575:ILE:HD13	2.49	0.41
1:B:65:LEU:HA	1:B:65:LEU:HD12	1.69	0.41
1:A:160:ASP:HA	1:A:218:LYS:HZ1	1.85	0.41
1:A:378:MSE:O	1:A:407:ALA:HB2	2.20	0.41
1:A:419:PRO:HA	1:A:422:PHE:CZ	2.55	0.41
1:A:551:GLU:HA	1:A:552:THR:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:489:ASN:O	1:B:493:ILE:HG23	2.21	0.41
1:B:492:GLN:CD	1:B:575:ILE:HD13	2.39	0.41
1:A:167:TRP:CG	1:A:173:ARG:HD2	2.56	0.41
1:A:456:VAL:O	1:A:456:VAL:HG23	2.21	0.41
1:B:335:PRO:HG2	1:B:337:ARG:NH1	2.36	0.41
1:A:152:ALA:HB1	1:A:165:LEU:HD22	2.02	0.41
1:A:332:ARG:HH21	1:A:343:PHE:CB	2.27	0.41
1:A:439:GLY:HA2	1:A:440:THR:O	2.20	0.41
1:B:252:LEU:HD23	1:B:299:TYR:CE1	2.56	0.41
1:B:449:VAL:HG12	1:B:450:ASP:OD2	2.21	0.41
1:A:206:GLY:C	1:A:208:ALA:H	2.23	0.41
1:A:286:THR:HG22	1:A:287:GLY:N	2.35	0.41
1:A:269:TYR:HD1	1:A:298:TYR:CD1	2.38	0.41
1:A:548:GLN:HB3	1:A:549:THR:H	1.53	0.41
1:B:578:ASP:OD2	1:B:582:TYR:N	2.54	0.41
1:B:261:GLU:HG2	1:B:262:PHE:CD1	2.56	0.41
1:B:269:TYR:HB3	1:B:299:TYR:HE2	1.86	0.41
1:B:564:ALA:HA	1:B:567:ARG:NE	2.36	0.41
1:A:178:ARG:HH12	1:A:340:VAL:HG23	1.85	0.40
1:B:302:ALA:HA	1:B:369:ASP:OD2	2.21	0.40
1:B:91:GLY:O	1:B:94:LYS:HG2	2.21	0.40
1:A:180:TYR:HA	3:A:843:HOH:O	2.21	0.40
1:A:227:LEU:HD12	1:A:227:LEU:HA	1.72	0.40
1:A:546:PHE:O	1:A:575:ILE:HG13	2.22	0.40
1:B:522:ALA:O	1:B:526:LEU:HA	2.21	0.40
1:A:214:THR:HB	1:A:337:ARG:HD3	2.04	0.40
1:B:445:PRO:HA	1:B:465:LYS:HE3	2.03	0.40
1:A:506:TRP:HB3	1:A:543:TYR:CE2	2.56	0.40

All (1) 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)
3:B:874:HOH:O	3:B:878:HOH:O[1_556]	2.01	0.19

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	593/603 (98%)	472 (80%)	91 (15%)	30 (5%)	2	6
1	B	593/603 (98%)	472 (80%)	92 (16%)	29 (5%)	2	7
All	All	1186/1206 (98%)	944 (80%)	183 (15%)	59 (5%)	2	6

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	THR
1	A	216	THR
1	A	287	GLY
1	A	323	LYS
1	A	324	TYR
1	A	353	GLU
1	A	410	THR
1	A	454	ALA
1	A	504	PRO
1	A	513	SER
1	B	102	ASN
1	B	258	ILE
1	B	259	SER
1	B	410	THR
1	B	439	GLY
1	B	474	MSE
1	B	509	ALA
1	B	536	SER
1	A	204	ASP
1	A	348	VAL
1	A	436	MSE
1	A	455	LEU
1	A	458	ASP
1	A	467	LYS
1	A	521	VAL

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Mol	Chain	Res	Type
1	A	552	THR
1	A	580	ASP
1	B	190	ASN
1	B	256	LEU
1	B	500	LEU
1	B	504	PRO
1	B	537	GLN
1	A	321	ALA
1	A	440	THR
1	A	551	GLU
1	B	338	ALA
1	B	348	VAL
1	B	350	SER
1	B	467	LYS
1	B	505	ALA
1	B	551	GLU
1	A	335	PRO
1	A	459	ASN
1	B	289	SER
1	B	316	ALA
1	B	321	ALA
1	B	335	PRO
1	B	454	ALA
1	A	316	ALA
1	A	350	SER
1	A	553	ALA
1	B	286	THR
1	B	570	ILE
1	A	236	SER
1	B	236	SER
1	B	456	VAL
1	A	340	VAL
1	A	527	GLY
1	B	527	GLY

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	518/517 (100%)	490 (95%)	28 (5%)	22	53
1	B	518/517 (100%)	488 (94%)	30 (6%)	20	50
All	All	1036/1034 (100%)	978 (94%)	58 (6%)	21	51

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	72	CYS
1	A	95	ASN
1	A	116	ASN
1	A	146	LYS
1	A	160	ASP
1	A	204	ASP
1	A	212	ARG
1	A	229	SER
1	A	253	TYR
1	A	257	ASN
1	A	286	THR
1	A	288	LYS
1	A	303	ARG
1	A	317	LEU
1	A	330	CYS
1	A	332	ARG
1	A	373	PHE
1	A	450	ASP
1	A	453	SER
1	A	455	LEU
1	A	467	LYS
1	A	470	GLN
1	A	473	LYS
1	A	502	ARG
1	A	508	LYS
1	A	516	ASN
1	A	528	LEU
1	A	582	TYR
1	B	0	SER
1	B	11	GLN
1	B	95	ASN
1	B	100	SER
1	B	189	LYS
1	B	199	THR
1	B	218	LYS

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Mol	Chain	Res	Type
1	B	229	SER
1	B	260	ASP
1	B	288	LYS
1	B	303	ARG
1	B	310	SER
1	B	323	LYS
1	B	330	CYS
1	B	332	ARG
1	B	373	PHE
1	B	435	ASP
1	B	437	PHE
1	B	438	LEU
1	B	464	HIS
1	B	497	ARG
1	B	499	PHE
1	B	510	VAL
1	B	518	GLN
1	B	542	ASP
1	B	543	TYR
1	B	567	ARG
1	B	573	LEU
1	B	582	TYR
1	B	583	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	492	GLN
1	A	548	GLN
1	B	11	GLN
1	B	519	ASN
1	B	554	HIS

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](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th 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	589/603 (97%)	0.98	103 (17%) 1 1	32, 73, 173, 206	0
1	B	589/603 (97%)	1.03	122 (20%) 1 0	33, 71, 175, 208	0
All	All	1178/1206 (97%)	1.00	225 (19%) 1 1	32, 72, 174, 208	0

All (225) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	596	ASN	13.9
1	A	335	PRO	11.7
1	A	347	LYS	11.1
1	A	342	CYS	10.5
1	B	593	PRO	10.4
1	A	587	PHE	9.6
1	A	583	ASP	8.7
1	B	506	TRP	8.3
1	B	501	THR	8.0
1	B	573	LEU	7.9
1	A	457	TYR	7.6
1	A	344	ASP	7.4
1	B	476	TYR	7.3
1	A	593	PRO	7.2
1	B	485	SER	7.1
1	B	527	GLY	7.0
1	B	543	TYR	6.8
1	A	490	ARG	6.7
1	B	544	VAL	6.6
1	B	594	ARG	6.6
1	B	595	ARG	6.5
1	B	592	ILE	6.5
1	B	550	THR	6.5
1	A	345	LYS	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	544	VAL	6.4
1	A	455	LEU	6.4
1	B	588	THR	6.3
1	B	495	VAL	6.3
1	A	350	SER	6.3
1	B	545	ILE	6.2
1	A	348	VAL	6.1
1	B	350	SER	6.1
1	B	487	ALA	6.0
1	B	589	SER	5.9
1	B	505	ALA	5.9
1	A	464	HIS	5.9
1	A	586	GLN	5.9
1	A	346	PHE	5.8
1	A	500	LEU	5.7
1	A	505	ALA	5.7
1	A	475	PHE	5.6
1	A	466	ASP	5.5
1	A	476	TYR	5.5
1	A	596	ASN	5.4
1	A	548	GLN	5.4
1	A	343	PHE	5.4
1	A	498	GLU	5.4
1	A	595	ARG	5.3
1	B	587	PHE	5.3
1	A	506	TRP	5.3
1	B	584	LYS	5.2
1	B	583	ASP	5.2
1	B	343	PHE	5.2
1	A	528	LEU	5.2
1	A	547	THR	5.1
1	B	531	GLN	5.1
1	A	594	ARG	5.1
1	B	342	CYS	5.1
1	B	509	ALA	5.1
1	B	561	PHE	5.0
1	B	346	PHE	5.0
1	B	497	ARG	5.0
1	A	334	ILE	5.0
1	B	486	SER	4.9
1	B	574	CYS	4.9
1	A	588	THR	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	550	THR	4.8
1	B	520	ALA	4.7
1	A	510	VAL	4.7
1	B	455	LEU	4.7
1	B	530	THR	4.6
1	B	475	PHE	4.6
1	A	341	GLU	4.5
1	A	574	CYS	4.5
1	A	546	PHE	4.5
1	B	546	PHE	4.4
1	A	338	ALA	4.4
1	B	463	ALA	4.3
1	A	502	ARG	4.3
1	A	485	SER	4.3
1	A	491	PRO	4.3
1	B	345	LYS	4.3
1	B	517	SER	4.2
1	B	493	ILE	4.2
1	B	347	LYS	4.2
1	B	547	THR	4.2
1	A	499	PHE	4.2
1	A	561	PHE	4.2
1	A	349	ASN	4.2
1	A	337	ARG	4.2
1	A	509	ALA	4.1
1	B	494	GLY	4.1
1	B	564	ALA	4.1
1	A	339	ARG	4.1
1	B	548	GLN	4.1
1	A	575	ILE	4.0
1	B	586	GLN	4.0
1	A	524	LYS	4.0
1	B	340	VAL	4.0
1	B	348	VAL	3.9
1	B	456	VAL	3.9
1	B	496	VAL	3.9
1	A	568	ALA	3.9
1	B	521	VAL	3.9
1	B	349	ASN	3.9
1	A	570	ILE	3.9
1	A	511	PHE	3.9
1	B	504	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	484	VAL	3.8
1	B	341	GLU	3.8
1	A	579	ARG	3.8
1	A	507	ARG	3.8
1	B	502	ARG	3.8
1	B	351	THR	3.7
1	B	503	ASN	3.7
1	B	333	ILE	3.7
1	A	463	ALA	3.6
1	B	500	LEU	3.6
1	B	572	ILE	3.6
1	B	549	THR	3.6
1	B	579	ARG	3.6
1	B	580	ASP	3.6
1	A	520	ALA	3.6
1	A	592	ILE	3.6
1	B	585	LEU	3.6
1	B	590	LEU	3.6
1	B	498	GLU	3.6
1	B	528	LEU	3.6
1	B	344	ASP	3.6
1	B	466	ASP	3.5
1	A	488	ILE	3.5
1	B	508	LYS	3.5
1	B	523	SER	3.5
1	A	517	SER	3.5
1	B	570	ILE	3.5
1	A	480	ILE	3.4
1	A	590	LEU	3.4
1	B	472	PHE	3.4
1	B	591	GLU	3.3
1	A	573	LEU	3.2
1	B	336	ALA	3.2
1	B	335	PRO	3.2
1	A	571	GLY	3.2
1	B	575	ILE	3.1
1	A	521	VAL	3.1
1	A	295	LEU	3.1
1	A	493	ILE	3.1
1	B	563	VAL	3.1
1	B	471	CYS	3.1
1	B	479	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	541	TYR	3.0
1	A	489	ASN	3.0
1	B	511	PHE	3.0
1	A	589	SER	3.0
1	B	512	ILE	3.0
1	A	492	GLN	2.9
1	B	483	ASP	2.9
1	A	567	ARG	2.9
1	A	523	SER	2.9
1	B	491	PRO	2.9
1	B	480	ILE	2.9
1	A	542	ASP	2.9
1	B	19	CYS	2.8
1	A	591	GLU	2.8
1	B	551	GLU	2.8
1	B	515	TYR	2.8
1	B	514	PRO	2.8
1	B	582	TYR	2.8
1	B	477	LYS	2.7
1	B	499	PHE	2.7
1	A	442	ARG	2.7
1	B	462	LYS	2.7
1	A	549	THR	2.7
1	B	465	LYS	2.7
1	A	512	ILE	2.6
1	A	563	VAL	2.6
1	A	545	ILE	2.6
1	B	467	LYS	2.6
1	A	522	ALA	2.6
1	A	564	ALA	2.6
1	B	522	ALA	2.6
1	A	580	ASP	2.5
1	A	584	LYS	2.5
1	A	565	ILE	2.5
1	A	447	GLU	2.5
1	A	572	ILE	2.5
1	B	461	LEU	2.4
1	B	510	VAL	2.4
1	A	497	ARG	2.4
1	B	247	VAL	2.4
1	B	538	GLY	2.4
1	B	16	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	526	LEU	2.4
1	B	252	LEU	2.4
1	B	558	VAL	2.4
1	A	446	ALA	2.3
1	A	462	LYS	2.3
1	B	464	HIS	2.3
1	B	446	ALA	2.3
1	B	565	ILE	2.3
1	B	468	SER	2.3
1	A	336	ALA	2.3
1	A	471	CYS	2.3
1	B	214	THR	2.2
1	B	285	GLY	2.2
1	A	479	VAL	2.2
1	A	437	PHE	2.2
1	B	529	PRO	2.2
1	A	252	LEU	2.2
1	B	490	ARG	2.2
1	B	568	ALA	2.2
1	B	473	LYS	2.1
1	A	205	TYR	2.1
1	A	578	ASP	2.1
1	B	426	CYS	2.1
1	B	457	TYR	2.1
1	B	518	GLN	2.1
1	B	556	CYS	2.1
1	A	534	ASP	2.1
1	A	197	GLU	2.1
1	A	325	LEU	2.0
1	B	447	GLU	2.0
1	A	270	GLN	2.0
1	B	533	VAL	2.0
1	A	303	ARG	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](#)

There are no monosaccharides in this entry.

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, 95th 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
2	ZN	B	703	1/1	0.96	0.39	337,337,337,337	0
2	ZN	B	702	1/1	0.98	0.22	109,109,109,109	0
2	ZN	A	702	1/1	0.98	0.20	77,77,77,77	0
2	ZN	A	701	1/1	0.98	0.22	54,54,54,54	0
2	ZN	B	701	1/1	0.99	0.20	50,50,50,50	0
2	ZN	A	703	1/1	1.00	0.19	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.