Full wwPDB X-ray Structure Validation Report

Sep 13, 2020 – 01:59 PM BST

PDB ID	:	3ZZH
Title	:	Crystal structure of the amino acid kinase domain from Saccharomyces cerevisiae acetylglutamate kinase in complex with its feed- back inhibitor L-arginine
Authors	:	de Cima, S.; Gil-Ortiz, F.; Crabeel, M.; Fita, I.; Rubio, V.
Deposited on	:	2011-09-01
Resolution	:	2.10 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 following versions of software and data (see references (1)) were used in the production of this report:

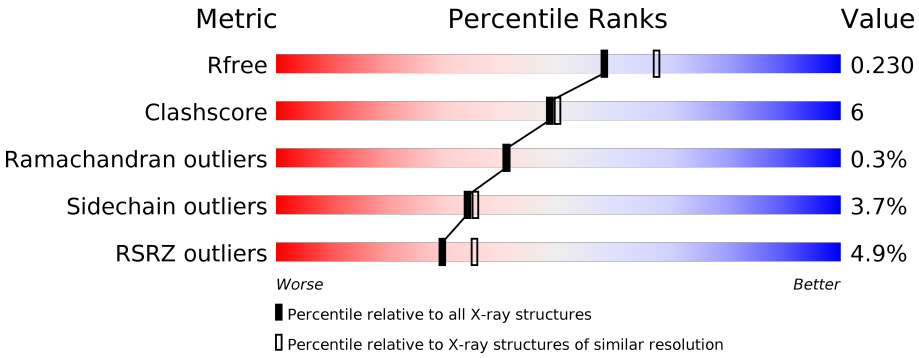
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.4.dev1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4.dev1

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=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	307	4% 85% 9% • 5%
1	B	307	2% 85% 7% • 6%
1	C	307	9% 84% 9% • 6%
1	D	307	5% 82% 11% • 6%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	B	1362	-	-	X	-
2	EDO	C	1357	-	-	X	-
2	EDO	D	1358	-	-	X	-
2	EDO	D	1363	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 9832 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 ACETYLGLUTAMATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	0	3	0
			2274	1443	387	436	8			
1	B	289	Total	C	N	O	S	0	3	0
			2259	1434	382	435	8			
1	C	288	Total	C	N	O	S	0	3	0
			2251	1429	379	436	7			
1	D	289	Total	C	N	O	S	0	5	0
			2275	1443	385	439	8			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	MET	-	expression tag	UNP Q01217
A	51	GLY	-	expression tag	UNP Q01217
A	52	HIS	-	expression tag	UNP Q01217
A	53	HIS	-	expression tag	UNP Q01217
A	54	HIS	-	expression tag	UNP Q01217
A	55	HIS	-	expression tag	UNP Q01217
A	56	HIS	-	expression tag	UNP Q01217
A	57	HIS	-	expression tag	UNP Q01217
B	50	MET	-	expression tag	UNP Q01217
B	51	GLY	-	expression tag	UNP Q01217
B	52	HIS	-	expression tag	UNP Q01217
B	53	HIS	-	expression tag	UNP Q01217
B	54	HIS	-	expression tag	UNP Q01217
B	55	HIS	-	expression tag	UNP Q01217
B	56	HIS	-	expression tag	UNP Q01217
B	57	HIS	-	expression tag	UNP Q01217
C	50	MET	-	expression tag	UNP Q01217
C	51	GLY	-	expression tag	UNP Q01217
C	52	HIS	-	expression tag	UNP Q01217
C	53	HIS	-	expression tag	UNP Q01217
C	54	HIS	-	expression tag	UNP Q01217

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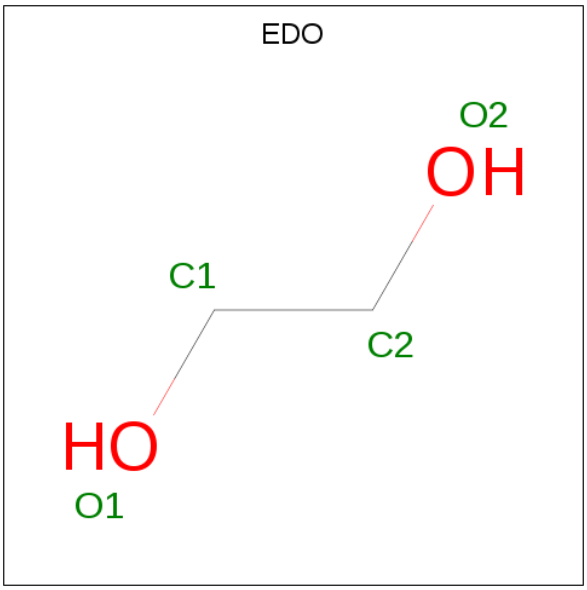
Chain	Residue	Modelled	Actual	Comment	Reference
C	55	HIS	-	expression tag	UNP Q01217
C	56	HIS	-	expression tag	UNP Q01217
C	57	HIS	-	expression tag	UNP Q01217
D	50	MET	-	expression tag	UNP Q01217
D	51	GLY	-	expression tag	UNP Q01217
D	52	HIS	-	expression tag	UNP Q01217
D	53	HIS	-	expression tag	UNP Q01217
D	54	HIS	-	expression tag	UNP Q01217
D	55	HIS	-	expression tag	UNP Q01217
D	56	HIS	-	expression tag	UNP Q01217
D	57	HIS	-	expression tag	UNP Q01217

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0

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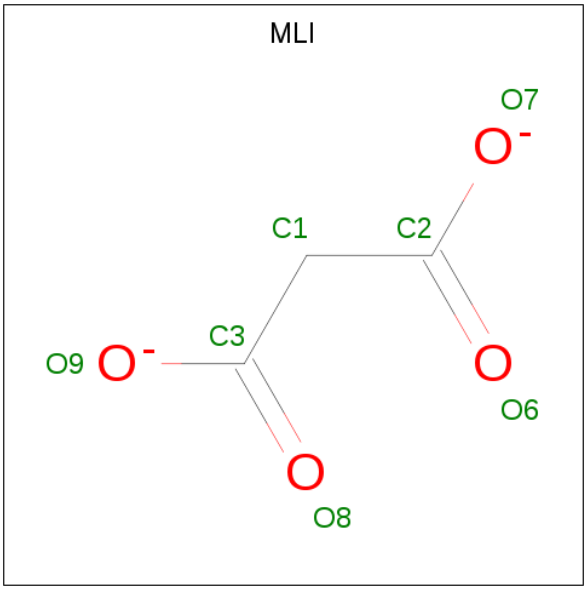
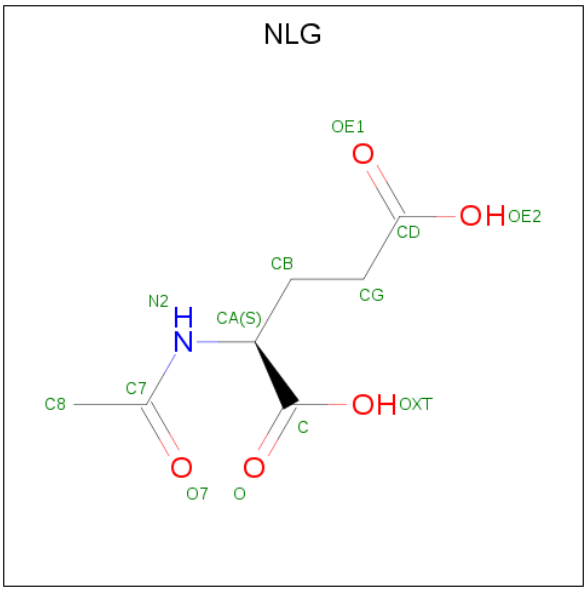
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	D	2	Total Cl 2 2	0	0
3	C	1	Total Cl 1 1	0	0

- Molecule 4 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



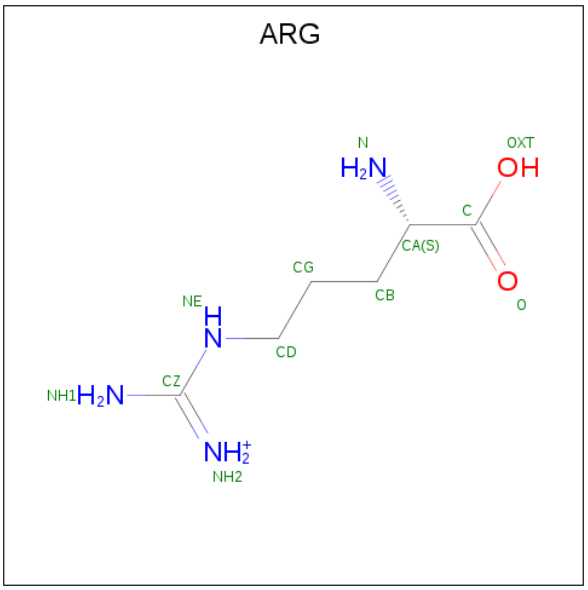
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 3 4	0	0
4	B	1	Total C O 7 3 4	0	0
4	D	1	Total C O 7 3 4	0	0

- Molecule 5 is N-ACETYL-L-GLUTAMATE (three-letter code: NLG) (formula: $C_7H_{11}NO_5$).



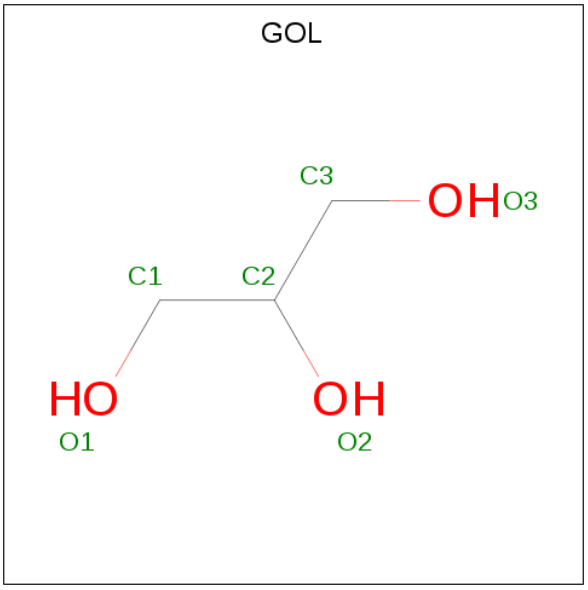
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 13 7 1 5	0	0
5	B	1	Total C N O 13 7 1 5	0	0
5	C	1	Total C N O 13 7 1 5	0	0
5	D	1	Total C N O 13 7 1 5	0	0

- Molecule 6 is ARGININE (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			12	6	4	2		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is water.

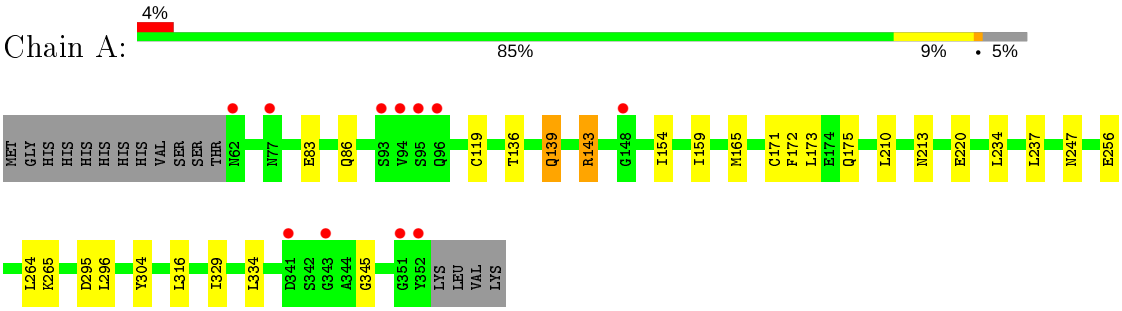
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	123	Total	O	0	0
			123	123		
8	B	144	Total	O	0	0
			144	144		
8	C	91	Total	O	0	0
			91	91		
8	D	139	Total	O	0	0
			139	139		

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.

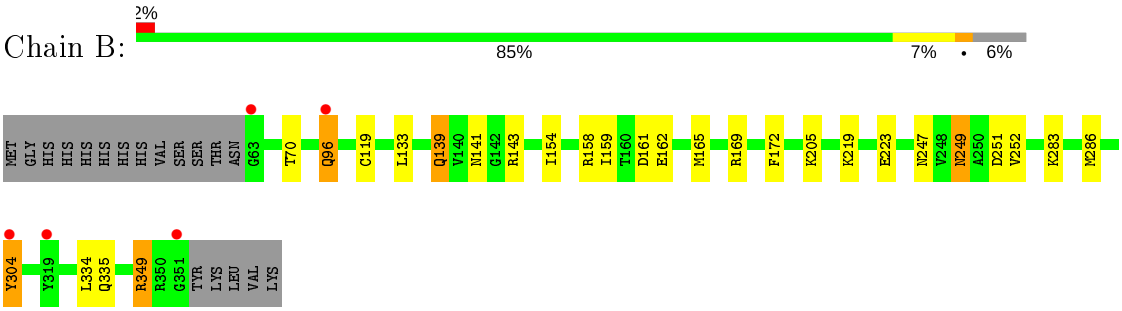
- Molecule 1: ACETYLGLUTAMATE KINASE

Chain A:



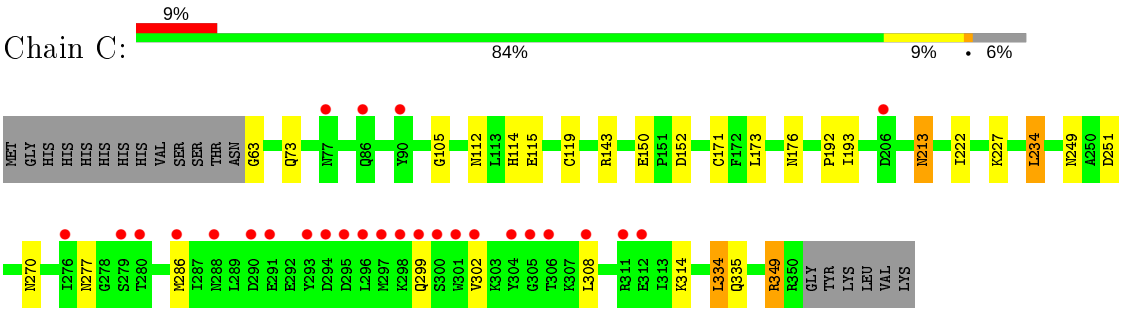
- Molecule 1: ACETYLGLUTAMATE KINASE

Chain B:



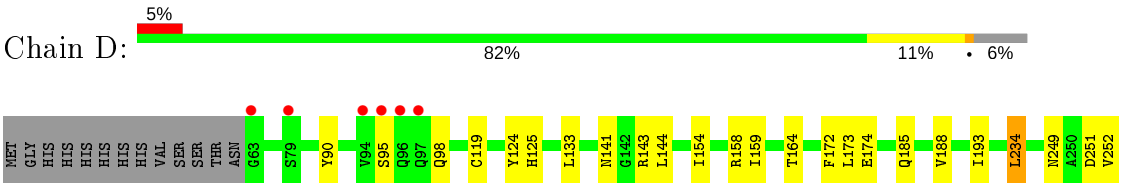
- Molecule 1: ACETYLGLUTAMATE KINASE

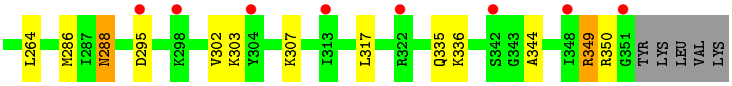
Chain C:



- Molecule 1: ACETYLGLUTAMATE KINASE

Chain D:




L264
M286
I287
N288
D295
K298
V302
K303
Y304
K307
I313
L317
R322
Q335
K336
S342
G343
A344
I348
R349
R350
G351
TYR
LYS
LEU
VAL
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.49Å 99.60Å 189.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 24.43 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-2.10) 99.3 (24.43-2.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.55 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.180 , 0.215 0.194 , 0.230	Depositor DCC
R_{free} test set	3869 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	19.7	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 46.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9832	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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: GOL, MLI, EDO, NLG, CL

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	0.34	0/2307	0.52	0/3118
1	B	0.37	0/2291	0.53	0/3097
1	C	0.35	0/2283	0.52	0/3088
1	D	0.35	0/2307	0.54	0/3117
All	All	0.35	0/9188	0.53	0/12420

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2274	0	2323	17	0
1	B	2259	0	2305	24	0
1	C	2251	0	2289	31	0
1	D	2275	0	2325	33	0
2	A	24	0	36	5	0
2	B	64	0	96	17	0
2	C	32	0	48	16	0
2	D	60	0	90	19	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
4	A	7	0	2	0	0
4	B	7	0	2	1	0
4	D	7	0	2	0	0
5	A	13	0	9	0	0
5	B	13	0	9	0	0
5	C	13	0	9	0	0
5	D	13	0	9	0	0
6	C	12	0	12	0	0
7	C	6	0	8	0	0
8	A	123	0	0	0	0
8	B	144	0	0	6	0
8	C	91	0	0	2	0
8	D	139	0	0	2	0
All	All	9832	0	9574	114	0

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 6.

All (114) 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:D:119[B]:CYS:SG	1:D:335[B]:GLN:NE2	2.06	1.29
1:D:185:GLN:HE21	2:D:1363:EDO:C1	1.75	0.99
1:B:119[B]:CYS:SG	1:B:335[B]:GLN:NE2	2.35	0.99
1:A:119[B]:CYS:SG	1:A:334:LEU:HD23	2.07	0.93
1:C:173:LEU:HD11	2:C:1357:EDO:H22	1.54	0.87
2:B:1364:EDO:H22	8:B:2142:HOH:O	1.78	0.82
1:C:105:GLY:HA3	2:C:1353:EDO:H21	1.65	0.78
1:C:119:CYS:SG	1:C:334:LEU:HD12	2.23	0.78
1:C:173:LEU:HD11	2:C:1357:EDO:C2	2.13	0.78
1:A:139:GLN:HG3	1:A:175:GLN:NE2	2.00	0.77
1:C:227:LYS:CE	2:D:1363:EDO:H22	2.16	0.75
1:D:185:GLN:HE21	2:D:1363:EDO:H11	1.51	0.75
1:D:185:GLN:NE2	2:D:1363:EDO:C1	2.50	0.75
2:D:1364:EDO:H22	8:D:2028:HOH:O	1.85	0.74
2:B:1364:EDO:H21	8:B:2038:HOH:O	1.87	0.73
1:B:283:LYS:NZ	2:B:1362:EDO:H22	2.03	0.73
1:C:173:LEU:HD21	2:C:1357:EDO:H21	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:ASN:HD21	1:D:251:ASP:HB2	1.54	0.72
1:C:63:GLY:N	2:C:1355:EDO:HO1	1.86	0.72
1:A:304:TYR:HA	2:A:1356:EDO:H12	1.74	0.69
1:B:162:GLU:HG3	2:B:1360:EDO:H21	1.75	0.67
1:C:222:ILE:HD11	1:C:234:LEU:HD11	1.75	0.67
1:B:249:ASN:HD21	1:B:251:ASP:HB2	1.59	0.66
1:D:335[B]:GLN:HA	1:D:335[B]:GLN:OE1	1.95	0.66
1:C:193:ILE:HB	1:C:234:LEU:HD22	1.77	0.65
1:D:185:GLN:NE2	2:D:1363:EDO:H12	2.12	0.65
1:A:165:MET:HE1	1:A:247:ASN:HB2	1.80	0.63
1:C:227:LYS:HE2	2:D:1363:EDO:H22	1.79	0.63
1:D:288:ASN:HD22	1:D:288:ASN:C	2.01	0.63
1:B:161:ASP:HB2	2:B:1360:EDO:H12	1.81	0.63
1:A:143:ARG:NH1	1:A:171:CYS:SG	2.71	0.62
1:D:154:ILE:CG1	1:D:159:ILE:HD11	2.30	0.62
2:B:1362:EDO:H21	8:B:2135:HOH:O	1.99	0.62
1:A:256:GLU:OE2	2:A:1358:EDO:H22	2.00	0.61
1:B:283:LYS:HZ2	2:B:1362:EDO:H22	1.63	0.60
1:B:139:GLN:H	1:B:139:GLN:HE21	1.47	0.60
1:D:154:ILE:HD11	1:D:159:ILE:HD11	1.84	0.60
2:B:1364:EDO:H12	8:B:2099:HOH:O	2.00	0.60
1:C:249:ASN:HD21	1:C:251:ASP:HB2	1.67	0.59
1:D:185:GLN:HE21	2:D:1363:EDO:H12	1.61	0.59
1:A:264:LEU:HD12	1:A:265:LYS:HE2	1.84	0.58
1:B:335[B]:GLN:HA	1:B:335[B]:GLN:OE1	2.04	0.58
1:C:152:ASP:OD1	2:C:1351:EDO:H21	2.04	0.58
2:D:1364:EDO:H12	8:D:2137:HOH:O	2.03	0.57
1:C:270:ASN:HA	2:C:1353:EDO:H22	1.85	0.57
1:D:154:ILE:HG13	1:D:159:ILE:HD11	1.85	0.57
1:D:249:ASN:ND2	1:D:251:ASP:HB2	2.20	0.56
1:C:114:HIS:HB2	2:C:1354:EDO:H21	1.87	0.55
1:B:169:ARG:HE	2:B:1352:EDO:H22	1.72	0.54
1:D:154:ILE:CD1	1:D:159:ILE:HD11	2.38	0.54
1:D:144:LEU:HD13	2:D:1358:EDO:H21	1.90	0.54
1:C:112:ASN:ND2	2:C:1354:EDO:O2	2.42	0.53
1:D:317:LEU:HD13	1:D:349:ARG:HA	1.90	0.53
1:D:185:GLN:NE2	2:D:1363:EDO:H11	2.19	0.53
2:C:1352:EDO:H12	8:C:2049:HOH:O	2.09	0.53
1:D:344:ALA:C	2:D:1362:EDO:H22	2.30	0.52
1:B:249:ASN:ND2	1:B:251:ASP:HB2	2.24	0.52
1:D:164:THR:HG21	2:D:1358:EDO:H22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:GLN:HB3	1:C:335:GLN:HE22	1.74	0.51
1:A:83:GLU:HA	1:A:86:GLN:HE21	1.75	0.51
1:D:193:ILE:HB	1:D:234:LEU:HD22	1.93	0.51
1:B:165:MET:HE1	1:B:247:ASN:HB2	1.92	0.51
1:D:164:THR:CG2	2:D:1358:EDO:H22	2.41	0.51
1:B:154:ILE:HG13	1:B:159:ILE:HD11	1.92	0.51
1:C:114:HIS:HB2	2:C:1354:EDO:C2	2.41	0.50
1:C:249:ASN:ND2	1:C:251:ASP:HB2	2.26	0.50
1:D:302:VAL:HG12	1:D:307:LYS:HG3	1.93	0.50
1:C:227:LYS:NZ	2:D:1363:EDO:H22	2.26	0.50
2:B:1366:EDO:H22	8:B:2098:HOH:O	2.12	0.49
1:D:144:LEU:CD1	2:D:1358:EDO:H21	2.43	0.49
1:D:141:ASN:ND2	1:D:158:ARG:HH12	2.11	0.49
1:D:344:ALA:CA	2:D:1362:EDO:H22	2.43	0.48
1:D:119[B]:CYS:SG	1:D:335[B]:GLN:CD	2.86	0.48
1:C:286:MET:HE1	1:C:349:ARG:HD3	1.95	0.48
1:C:173:LEU:HD11	2:C:1357:EDO:H21	1.95	0.48
1:B:223:GLU:HA	2:B:1361:EDO:H22	1.96	0.47
1:B:143:ARG:NH2	8:B:2061:HOH:O	2.47	0.47
1:B:141:ASN:ND2	1:B:158:ARG:HH12	2.13	0.47
1:D:288:ASN:ND2	1:D:288:ASN:C	2.67	0.46
1:C:173:LEU:CD2	2:C:1357:EDO:H21	2.44	0.46
1:D:249:ASN:HD22	1:D:252:VAL:H	1.64	0.46
1:C:112:ASN:ND2	1:C:115[B]:GLU:OE1	2.49	0.45
1:C:150:GLU:O	2:C:1356:EDO:H22	2.17	0.45
1:C:176:ASN:OD1	1:C:192:PRO:HB3	2.17	0.45
1:C:152:ASP:OD2	2:C:1351:EDO:H21	2.17	0.45
1:A:173:LEU:HD12	2:B:1354:EDO:H11	1.99	0.44
1:A:256:GLU:OE2	2:A:1358:EDO:C2	2.64	0.44
1:D:125:HIS:HD1	2:D:1353:EDO:HO1	1.64	0.43
1:B:283:LYS:HZ3	2:B:1362:EDO:H22	1.77	0.43
1:B:141:ASN:HD21	1:B:158:ARG:HH12	1.66	0.43
1:C:152:ASP:CG	2:C:1351:EDO:H21	2.38	0.43
1:D:98:GLN:NE2	2:D:1365:EDO:C1	2.82	0.43
4:B:1368:MLI:O6	4:B:1368:MLI:O8	2.35	0.42
1:C:299:GLN:O	1:C:302:VAL:HG12	2.19	0.42
1:A:329:ILE:HG22	1:A:345:GLY:HA3	2.00	0.42
1:C:143:ARG:HG3	1:C:171:CYS:SG	2.60	0.42
1:A:154:ILE:HG13	1:A:159:ILE:HD11	2.02	0.42
1:C:234:LEU:HD23	1:C:234:LEU:N	2.35	0.42
1:A:264:LEU:O	1:A:264:LEU:HD13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:GLN:OE1	2:B:1361:EDO:H21	2.20	0.41
1:B:219:LYS:NZ	2:B:1358:EDO:O2	2.43	0.41
1:D:90:TYR:CE2	1:D:264:LEU:HD22	2.56	0.41
1:A:83:GLU:HA	1:A:86:GLN:NE2	2.34	0.41
1:D:124:TYR:CG	1:D:188:VAL:HG13	2.56	0.41
1:B:70:THR:OG1	2:B:1353:EDO:H12	2.21	0.41
1:A:304:TYR:CA	2:A:1356:EDO:H12	2.44	0.41
1:A:237:LEU:HD12	2:A:1353:EDO:H21	2.03	0.41
1:B:286:MET:SD	1:B:349:ARG:HD2	2.61	0.41
1:C:213:ASN:ND2	8:C:2068:HOH:O	2.54	0.41
1:B:70:THR:OG1	2:B:1353:EDO:C1	2.69	0.40
1:A:119[B]:CYS:SG	1:A:334:LEU:HB3	2.61	0.40
1:B:249:ASN:HD22	1:B:252:VAL:H	1.68	0.40
1:B:119[B]:CYS:SG	1:B:334:LEU:HD23	2.61	0.40
1:D:143:ARG:NH2	1:D:174:GLU:OE1	2.49	0.40

There are no symmetry-related clashes.

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	292/307 (95%)	283 (97%)	8 (3%)	1 (0%)	41	41
1	B	290/307 (94%)	283 (98%)	6 (2%)	1 (0%)	41	41
1	C	289/307 (94%)	282 (98%)	7 (2%)	0	100	100
1	D	292/307 (95%)	285 (98%)	6 (2%)	1 (0%)	41	41
All	All	1163/1228 (95%)	1133 (97%)	27 (2%)	3 (0%)	41	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	95	SER
1	A	136	THR
1	B	304	TYR

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	249/262 (95%)	239 (96%)	10 (4%)	31	32
1	B	247/262 (94%)	239 (97%)	8 (3%)	39	41
1	C	246/262 (94%)	239 (97%)	7 (3%)	43	47
1	D	250/262 (95%)	239 (96%)	11 (4%)	28	28
All	All	992/1048 (95%)	956 (96%)	36 (4%)	34	36

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	A	143	ARG
1	A	172	PHE
1	A	210	LEU
1	A	213	ASN
1	A	220	GLU
1	A	234	LEU
1	A	295	ASP
1	A	296	LEU
1	A	316	LEU
1	B	96	GLN
1	B	133	LEU
1	B	139	GLN
1	B	172	PHE
1	B	205	LYS
1	B	249	ASN
1	B	304	TYR
1	B	349	ARG
1	C	213	ASN

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Mol	Chain	Res	Type
1	C	234	LEU
1	C	277	ASN
1	C	308	LEU
1	C	314	LYS
1	C	334	LEU
1	C	349	ARG
1	D	133	LEU
1	D	172	PHE
1	D	173	LEU
1	D	234	LEU
1	D	286	MET
1	D	288	ASN
1	D	295	ASP
1	D	303	LYS
1	D	336	LYS
1	D	349	ARG
1	D	350	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	98	GLN
1	A	175	GLN
1	A	213	ASN
1	A	335	GLN
1	B	139	GLN
1	B	141	ASN
1	B	213	ASN
1	B	249	ASN
1	B	332	GLN
1	C	76	ASN
1	C	112	ASN
1	C	213	ASN
1	C	249	ASN
1	C	277	ASN
1	C	332	GLN
1	C	335	GLN
1	D	98	GLN
1	D	141	ASN
1	D	185	GLN
1	D	249	ASN

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Mol	Chain	Res	Type
1	D	288	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 59 ligands modelled in this entry, 5 are monoatomic - leaving 54 for Mogul analysis.

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	NLG	B	1369	-	6,12,12	2.38	2 (33%)	7,15,15	0.91	0
4	MLI	A	1360	-	0,6,6	0.00	-	0,7,7	0.00	-
4	MLI	B	1368	-	0,6,6	0.00	-	0,7,7	0.00	-
5	NLG	A	1361	-	6,12,12	2.14	1 (16%)	7,15,15	1.26	1 (14%)
2	EDO	C	1355	-	3,3,3	0.48	0	2,2,2	0.32	0
2	EDO	A	1358	-	3,3,3	0.45	0	2,2,2	0.38	0
2	EDO	B	1363	-	3,3,3	0.47	0	2,2,2	0.35	0
2	EDO	B	1362	-	3,3,3	0.55	0	2,2,2	0.23	0
2	EDO	B	1351	-	3,3,3	0.51	0	2,2,2	0.24	0
2	EDO	D	1352	-	3,3,3	0.53	0	2,2,2	0.27	0
2	EDO	B	1366	-	3,3,3	0.54	0	2,2,2	0.29	0
2	EDO	C	1354	-	3,3,3	0.45	0	2,2,2	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	EDO	A	1357	-	3,3,3	0.48	0	2,2,2	0.24	0
2	EDO	C	1357	-	3,3,3	0.50	0	2,2,2	0.11	0
2	EDO	A	1353	-	3,3,3	0.70	0	2,2,2	0.19	0
2	EDO	D	1365	-	3,3,3	0.55	0	2,2,2	0.25	0
2	EDO	C	1352	-	3,3,3	0.74	0	2,2,2	0.20	0
2	EDO	D	1364	-	3,3,3	0.52	0	2,2,2	0.16	0
7	GOL	C	1359	-	5,5,5	0.60	0	5,5,5	0.44	0
2	EDO	A	1355	-	3,3,3	0.56	0	2,2,2	0.21	0
2	EDO	D	1361	-	3,3,3	0.60	0	2,2,2	0.24	0
2	EDO	A	1354	-	3,3,3	0.52	0	2,2,2	0.29	0
2	EDO	D	1358	-	3,3,3	0.44	0	2,2,2	0.39	0
2	EDO	D	1356	-	3,3,3	0.51	0	2,2,2	0.25	0
2	EDO	D	1363	-	3,3,3	0.42	0	2,2,2	0.28	0
2	EDO	B	1359	-	3,3,3	0.45	0	2,2,2	0.31	0
5	NLG	C	1361	-	6,12,12	2.00	1 (16%)	7,15,15	1.25	1 (14%)
2	EDO	B	1353	-	3,3,3	0.44	0	2,2,2	0.28	0
2	EDO	D	1360	-	3,3,3	0.48	0	2,2,2	0.28	0
2	EDO	C	1351	-	3,3,3	0.48	0	2,2,2	0.28	0
4	MLI	D	1369	-	0,6,6	0.00	-	0,7,7	0.00	-
2	EDO	D	1362	-	3,3,3	0.51	0	2,2,2	0.23	0
2	EDO	B	1360	-	3,3,3	0.51	0	2,2,2	0.27	0
2	EDO	D	1359	-	3,3,3	0.54	0	2,2,2	0.28	0
6	ARG	C	1362	-	7,11,11	0.51	0	6,13,13	0.43	0
2	EDO	B	1355	-	3,3,3	0.40	0	2,2,2	0.40	0
2	EDO	B	1358	-	3,3,3	0.42	0	2,2,2	0.44	0
2	EDO	C	1358	-	3,3,3	0.49	0	2,2,2	0.37	0
2	EDO	B	1357	-	3,3,3	0.48	0	2,2,2	0.34	0
2	EDO	C	1356	-	3,3,3	0.54	0	2,2,2	0.31	0
2	EDO	C	1353	-	3,3,3	0.44	0	2,2,2	0.28	0
2	EDO	B	1354	-	3,3,3	0.48	0	2,2,2	0.32	0
2	EDO	A	1356	-	3,3,3	0.58	0	2,2,2	0.21	0
2	EDO	D	1354	-	3,3,3	0.55	0	2,2,2	0.21	0
2	EDO	B	1364	-	3,3,3	0.55	0	2,2,2	0.17	0
2	EDO	D	1355	-	3,3,3	0.50	0	2,2,2	0.33	0
5	NLG	D	1370	-	6,12,12	2.34	2 (33%)	7,15,15	1.38	1 (14%)
2	EDO	B	1356	-	3,3,3	0.54	0	2,2,2	0.28	0
2	EDO	B	1352	-	3,3,3	0.57	0	2,2,2	0.32	0
2	EDO	B	1361	-	3,3,3	0.47	0	2,2,2	0.26	0
2	EDO	D	1353	-	3,3,3	0.43	0	2,2,2	0.25	0
2	EDO	B	1365	-	3,3,3	0.51	0	2,2,2	0.31	0
2	EDO	D	1366	-	3,3,3	0.45	0	2,2,2	0.32	0
2	EDO	D	1357	-	3,3,3	0.42	0	2,2,2	0.38	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	NLG	B	1369	-	-	0/7/13/13	-
4	MLI	A	1360	-	-	0/0/4/4	-
4	MLI	B	1368	-	-	0/0/4/4	-
5	NLG	A	1361	-	-	1/7/13/13	-
2	EDO	C	1355	-	-	1/1/1/1	-
2	EDO	A	1358	-	-	1/1/1/1	-
2	EDO	B	1363	-	-	1/1/1/1	-
2	EDO	B	1362	-	-	1/1/1/1	-
2	EDO	B	1351	-	-	0/1/1/1	-
2	EDO	D	1352	-	-	0/1/1/1	-
2	EDO	B	1366	-	-	1/1/1/1	-
2	EDO	C	1354	-	-	1/1/1/1	-
2	EDO	A	1357	-	-	1/1/1/1	-
2	EDO	C	1357	-	-	1/1/1/1	-
2	EDO	A	1353	-	-	1/1/1/1	-
2	EDO	D	1365	-	-	0/1/1/1	-
2	EDO	C	1352	-	-	1/1/1/1	-
2	EDO	D	1364	-	-	1/1/1/1	-
7	GOL	C	1359	-	-	4/4/4/4	-
2	EDO	A	1355	-	-	1/1/1/1	-
2	EDO	D	1361	-	-	0/1/1/1	-
2	EDO	A	1354	-	-	0/1/1/1	-
2	EDO	D	1358	-	-	1/1/1/1	-
2	EDO	D	1356	-	-	0/1/1/1	-
2	EDO	D	1363	-	-	0/1/1/1	-
2	EDO	B	1359	-	-	0/1/1/1	-
5	NLG	C	1361	-	-	0/7/13/13	-
2	EDO	B	1353	-	-	1/1/1/1	-
2	EDO	D	1360	-	-	1/1/1/1	-
2	EDO	C	1351	-	-	1/1/1/1	-
4	MLI	D	1369	-	-	0/0/4/4	-
2	EDO	D	1362	-	-	1/1/1/1	-
2	EDO	B	1360	-	-	0/1/1/1	-
2	EDO	D	1359	-	-	1/1/1/1	-
6	ARG	C	1362	-	-	0/7/11/11	-
2	EDO	B	1355	-	-	1/1/1/1	-
2	EDO	B	1358	-	-	1/1/1/1	-
2	EDO	C	1358	-	-	0/1/1/1	-
2	EDO	B	1357	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	C	1356	-	-	0/1/1/1	-
2	EDO	C	1353	-	-	1/1/1/1	-
2	EDO	B	1354	-	-	0/1/1/1	-
2	EDO	A	1356	-	-	1/1/1/1	-
2	EDO	D	1354	-	-	1/1/1/1	-
2	EDO	B	1364	-	-	1/1/1/1	-
2	EDO	D	1355	-	-	1/1/1/1	-
5	NLG	D	1370	-	-	0/7/13/13	-
2	EDO	B	1356	-	-	1/1/1/1	-
2	EDO	B	1352	-	-	0/1/1/1	-
2	EDO	B	1361	-	-	1/1/1/1	-
2	EDO	D	1353	-	-	1/1/1/1	-
2	EDO	B	1365	-	-	1/1/1/1	-
2	EDO	D	1366	-	-	0/1/1/1	-
2	EDO	D	1357	-	-	1/1/1/1	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	1370	NLG	C8-C7	-5.18	1.39	1.50
5	B	1369	NLG	C8-C7	-5.13	1.39	1.50
5	A	1361	NLG	C8-C7	-4.88	1.40	1.50
5	C	1361	NLG	C8-C7	-4.87	1.40	1.50
5	B	1369	NLG	CB-CA	2.43	1.56	1.53
5	D	1370	NLG	CB-CA	2.20	1.56	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	1370	NLG	O7-C7-C8	-2.57	117.28	122.06
5	A	1361	NLG	O7-C7-C8	-2.27	117.83	122.06
5	C	1361	NLG	CB-CA-N2	-2.22	106.96	110.19

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	1359	GOL	C1-C2-C3-O3
2	A	1357	EDO	O1-C1-C2-O2
7	C	1359	GOL	O1-C1-C2-C3
2	C	1355	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	B	1366	EDO	O1-C1-C2-O2
2	C	1354	EDO	O1-C1-C2-O2
2	C	1352	EDO	O1-C1-C2-O2
2	D	1364	EDO	O1-C1-C2-O2
2	A	1355	EDO	O1-C1-C2-O2
2	D	1358	EDO	O1-C1-C2-O2
2	B	1353	EDO	O1-C1-C2-O2
2	C	1351	EDO	O1-C1-C2-O2
2	B	1361	EDO	O1-C1-C2-O2
2	D	1353	EDO	O1-C1-C2-O2
2	D	1357	EDO	O1-C1-C2-O2
2	C	1357	EDO	O1-C1-C2-O2
2	D	1360	EDO	O1-C1-C2-O2
2	B	1357	EDO	O1-C1-C2-O2
2	C	1353	EDO	O1-C1-C2-O2
7	C	1359	GOL	O2-C2-C3-O3
2	D	1355	EDO	O1-C1-C2-O2
2	A	1358	EDO	O1-C1-C2-O2
2	B	1363	EDO	O1-C1-C2-O2
2	A	1353	EDO	O1-C1-C2-O2
2	B	1356	EDO	O1-C1-C2-O2
2	D	1362	EDO	O1-C1-C2-O2
2	B	1358	EDO	O1-C1-C2-O2
2	D	1354	EDO	O1-C1-C2-O2
2	B	1355	EDO	O1-C1-C2-O2
7	C	1359	GOL	O1-C1-C2-O2
5	A	1361	NLG	CA-CB-CG-CD
2	B	1362	EDO	O1-C1-C2-O2
2	D	1359	EDO	O1-C1-C2-O2
2	A	1356	EDO	O1-C1-C2-O2
2	B	1365	EDO	O1-C1-C2-O2
2	B	1364	EDO	O1-C1-C2-O2

There are no ring outliers.

26 monomers are involved in 58 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1368	MLI	1	0
2	C	1355	EDO	1	0
2	A	1358	EDO	2	0
2	B	1362	EDO	4	0
2	B	1366	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1354	EDO	3	0
2	C	1357	EDO	5	0
2	A	1353	EDO	1	0
2	D	1365	EDO	1	0
2	C	1352	EDO	1	0
2	D	1364	EDO	2	0
2	D	1358	EDO	4	0
2	D	1363	EDO	9	0
2	B	1353	EDO	2	0
2	C	1351	EDO	3	0
2	D	1362	EDO	2	0
2	B	1360	EDO	2	0
2	B	1358	EDO	1	0
2	C	1356	EDO	1	0
2	C	1353	EDO	2	0
2	B	1354	EDO	1	0
2	A	1356	EDO	2	0
2	B	1364	EDO	3	0
2	B	1352	EDO	1	0
2	B	1361	EDO	2	0
2	D	1353	EDO	1	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	291/307 (94%)	0.12	11 (3%) 40 46	9, 19, 40, 54	0
1	B	289/307 (94%)	-0.07	5 (1%) 70 74	8, 16, 31, 38	0
1	C	288/307 (93%)	0.43	27 (9%) 8 11	9, 20, 82, 115	0
1	D	289/307 (94%)	0.13	14 (4%) 30 36	7, 17, 36, 59	0
All	All	1157/1228 (94%)	0.15	57 (4%) 29 35	7, 18, 47, 115	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	96	GLN	9.7
1	D	94	VAL	8.3
1	C	302	VAL	6.5
1	C	296	LEU	6.5
1	A	94	VAL	6.0
1	A	352	TYR	5.9
1	C	301	TRP	5.8
1	D	63	GLY	5.7
1	C	295	ASP	5.5
1	C	291	GLU	5.3
1	C	300	SER	5.2
1	C	304	TYR	5.1
1	C	280	THR	4.8
1	B	63	GLY	4.7
1	A	341	ASP	4.6
1	C	305	GLY	4.6
1	D	95	SER	4.6
1	D	97	GLN	4.3
1	C	279	SER	4.2
1	A	96	GLN	4.2
1	B	304	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	351	GLY	3.9
1	C	86	GLN	3.9
1	C	299	GLN	3.8
1	C	293	TYR	3.7
1	C	290	ASP	3.6
1	C	306	THR	3.5
1	A	62	ASN	3.2
1	C	206	ASP	2.9
1	A	93	SER	2.9
1	B	319	TYR	2.9
1	B	96	GLN	2.9
1	C	294	ASP	2.7
1	C	288	ASN	2.6
1	A	343	GLY	2.6
1	D	348	ILE	2.6
1	A	148	GLY	2.6
1	C	90	TYR	2.5
1	D	342	SER	2.4
1	D	79	SER	2.4
1	D	322	ARG	2.4
1	D	351	GLY	2.3
1	D	295	ASP	2.3
1	C	298	LYS	2.3
1	C	311	ARG	2.3
1	A	77	ASN	2.3
1	D	304	TYR	2.3
1	B	351	GLY	2.2
1	C	276	ILE	2.1
1	D	313	ILE	2.1
1	C	297	MET	2.1
1	C	308	LEU	2.1
1	C	77	ASN	2.1
1	C	312[A]	GLU	2.1
1	D	298	LYS	2.1
1	A	95	SER	2.0
1	C	286	MET	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, 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
2	EDO	B	1356	4/4	0.48	0.25	51,52,52,52	0
2	EDO	D	1361	4/4	0.63	0.27	36,37,37,38	0
2	EDO	A	1353	4/4	0.66	0.36	31,33,33,33	0
4	MLI	A	1360	7/7	0.67	0.26	33,36,38,38	0
7	GOL	C	1359	6/6	0.69	0.24	35,36,36,37	0
2	EDO	C	1352	4/4	0.70	0.22	25,28,28,30	0
2	EDO	D	1362	4/4	0.71	0.35	53,53,53,53	0
2	EDO	B	1360	4/4	0.74	0.32	50,50,50,51	0
2	EDO	B	1358	4/4	0.75	0.22	45,46,46,46	0
2	EDO	B	1363	4/4	0.75	0.29	48,49,49,49	0
2	EDO	D	1366	4/4	0.76	0.35	36,37,37,38	0
2	EDO	D	1359	4/4	0.77	0.16	49,49,49,49	0
2	EDO	B	1361	4/4	0.77	0.27	51,52,52,52	0
2	EDO	A	1356	4/4	0.77	0.18	41,41,41,41	0
2	EDO	D	1352	4/4	0.78	0.26	32,32,33,33	0
2	EDO	D	1365	4/4	0.79	0.16	35,35,35,35	0
2	EDO	C	1354	4/4	0.79	0.32	42,42,42,42	0
2	EDO	D	1356	4/4	0.81	0.24	46,46,46,46	0
2	EDO	C	1351	4/4	0.81	0.16	32,34,35,36	0
2	EDO	B	1355	4/4	0.81	0.35	39,39,40,40	0
2	EDO	A	1358	4/4	0.81	0.15	41,41,42,42	0
2	EDO	D	1364	4/4	0.82	0.15	35,35,36,36	0
2	EDO	D	1354	4/4	0.82	0.20	41,42,42,42	0
4	MLI	B	1368	7/7	0.82	0.18	26,27,28,28	0
2	EDO	D	1360	4/4	0.82	0.28	38,40,40,40	0
2	EDO	B	1365	4/4	0.82	0.22	29,31,31,32	0
2	EDO	B	1357	4/4	0.82	0.13	51,51,51,52	0
2	EDO	D	1357	4/4	0.82	0.16	45,45,45,46	0
2	EDO	D	1355	4/4	0.83	0.32	33,34,34,34	0
2	EDO	C	1355	4/4	0.83	0.21	53,53,53,53	0
2	EDO	B	1352	4/4	0.84	0.28	20,22,23,24	0
2	EDO	A	1357	4/4	0.84	0.34	35,36,36,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	A	1354	4/4	0.84	0.19	48,49,49,49	0
2	EDO	B	1362	4/4	0.84	0.16	52,52,52,52	0
2	EDO	D	1363	4/4	0.84	0.31	34,35,35,36	0
2	EDO	C	1356	4/4	0.85	0.21	33,34,34,34	0
2	EDO	C	1357	4/4	0.85	0.27	27,28,29,29	0
2	EDO	B	1366	4/4	0.87	0.28	43,43,43,44	0
2	EDO	B	1364	4/4	0.87	0.20	32,32,34,35	0
2	EDO	D	1353	4/4	0.87	0.20	31,32,33,34	0
6	ARG	C	1362	12/12	0.88	0.11	28,28,30,30	0
2	EDO	B	1359	4/4	0.88	0.16	38,39,39,40	0
2	EDO	C	1358	4/4	0.89	0.15	45,45,45,45	0
2	EDO	A	1355	4/4	0.89	0.14	33,35,36,36	0
2	EDO	B	1354	4/4	0.90	0.16	44,45,45,45	0
4	MLI	D	1369	7/7	0.90	0.11	23,26,27,27	0
2	EDO	B	1353	4/4	0.92	0.17	29,31,31,33	0
2	EDO	C	1353	4/4	0.93	0.23	35,35,35,35	0
2	EDO	B	1351	4/4	0.94	0.09	24,26,26,26	0
3	CL	C	1360	1/1	0.94	0.05	36,36,36,36	0
5	NLG	B	1369	13/13	0.95	0.11	9,15,15,16	0
5	NLG	C	1361	13/13	0.95	0.09	12,13,14,14	0
5	NLG	A	1361	13/13	0.96	0.09	12,14,14,15	0
5	NLG	D	1370	13/13	0.96	0.09	10,15,17,18	0
2	EDO	D	1358	4/4	0.97	0.24	22,23,24,24	0
3	CL	A	1359	1/1	0.99	0.06	25,25,25,25	0
3	CL	D	1367	1/1	0.99	0.07	19,19,19,19	0
3	CL	D	1368	1/1	0.99	0.15	29,29,29,29	0
3	CL	B	1367	1/1	1.00	0.06	21,21,21,21	0

6.5 Other polymers (i)

There are no such residues in this entry.