Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 06:33 PM EDT

PDB ID	:	5OT0
Title	:	The thermostable L-asparaginase from Thermococcus kodakarensis
Authors	:	Guo, J.; Coker, A.R.; Wood, S.P.; Cooper, J.B.; Rashid, N.; Chohan, S.M.; Akhtar, M.
Deposited on	:	2017-08-18
Resolution	:	2.18 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 (i)) were used in the production of this report:

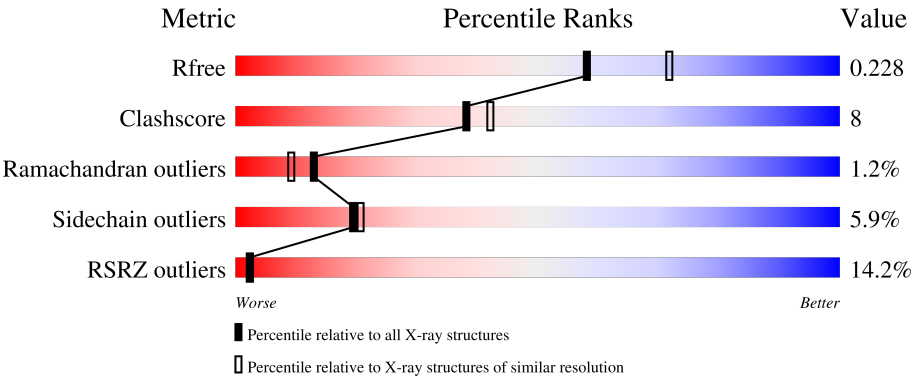
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.18 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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	328	2% 85% 12%
1	B	328	2% 86% 11%
1	C	328	2% 86% 12%
1	D	328	5% 87% 11%
1	E	328	22% 82% 15%

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Mol	Chain	Length	Quality of chain
1	F	328	

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
2	PO4	B	401	-	X	-	-
2	PO4	C	401	-	X	-	-
2	PO4	D	401	-	X	-	-
2	PO4	E	401	-	X	-	-

2 Entry composition (i)

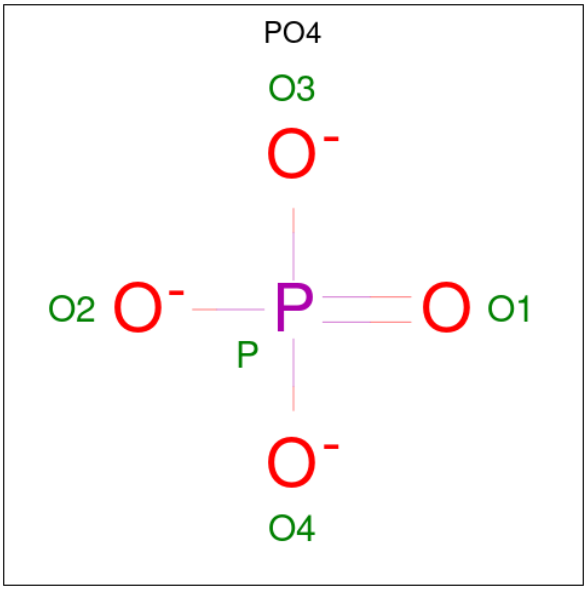
There are 5 unique types of molecules in this entry. The entry contains 15386 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-asparaginase.

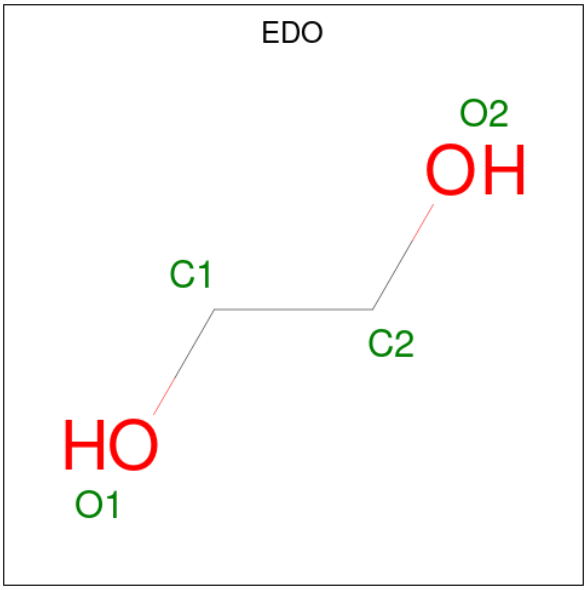
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	2	0
			2520	1595	441	474	10			
1	B	328	Total	C	N	O	S	0	3	0
			2523	1598	438	477	10			
1	C	328	Total	C	N	O	S	0	3	0
			2525	1598	442	475	10			
1	D	328	Total	C	N	O	S	0	1	0
			2510	1589	436	475	10			
1	E	328	Total	C	N	O	S	0	0	0
			2507	1587	436	474	10			
1	F	328	Total	C	N	O	S	0	1	0
			2514	1592	438	474	10			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



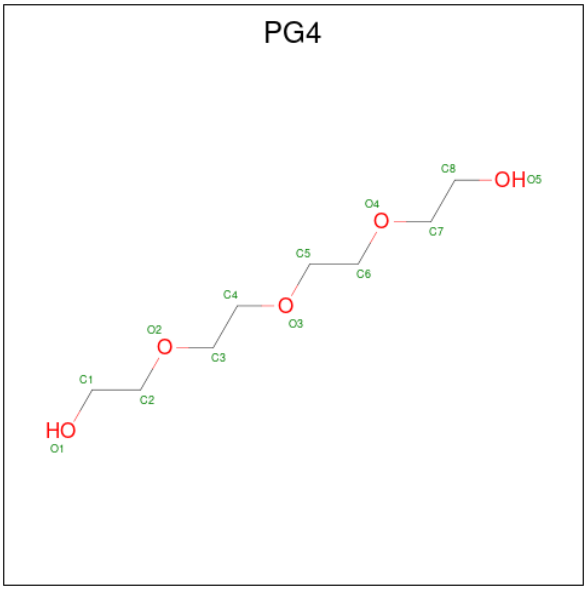
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 10 6 4	0	0

- Molecule 5 is water.

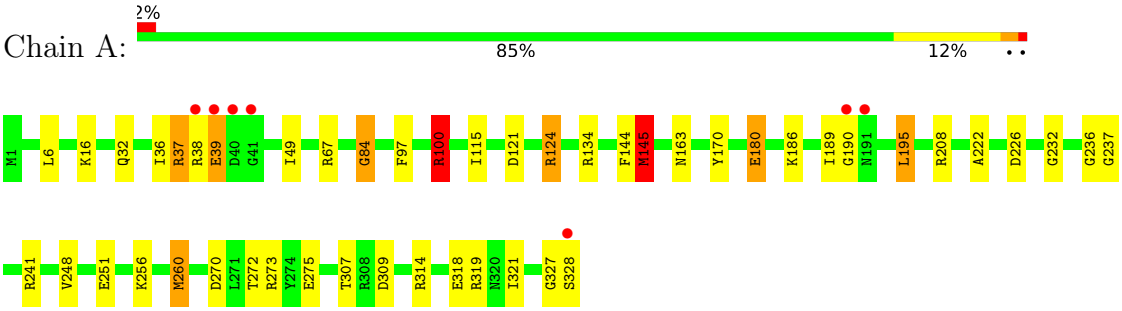
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	55	Total O 55 55	0	0
5	B	49	Total O 49 49	0	0
5	C	35	Total O 35 35	0	0
5	D	46	Total O 46 46	0	0
5	E	25	Total O 25 25	0	0
5	F	13	Total O 13 13	0	0

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.

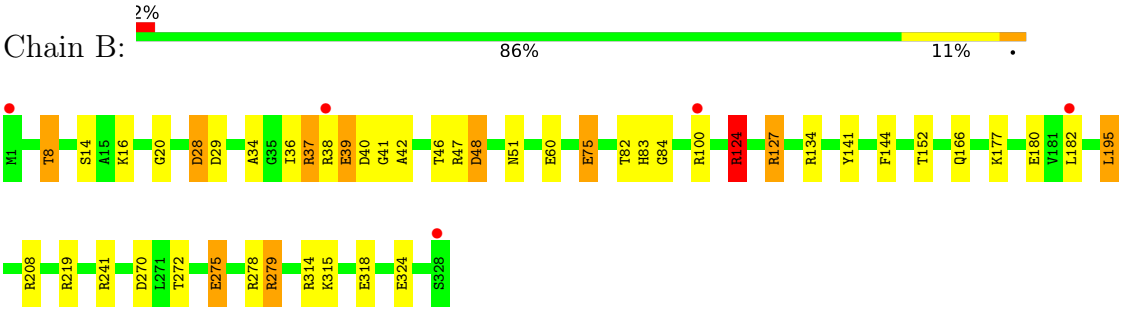
- Molecule 1: L-asparaginase

Chain A:



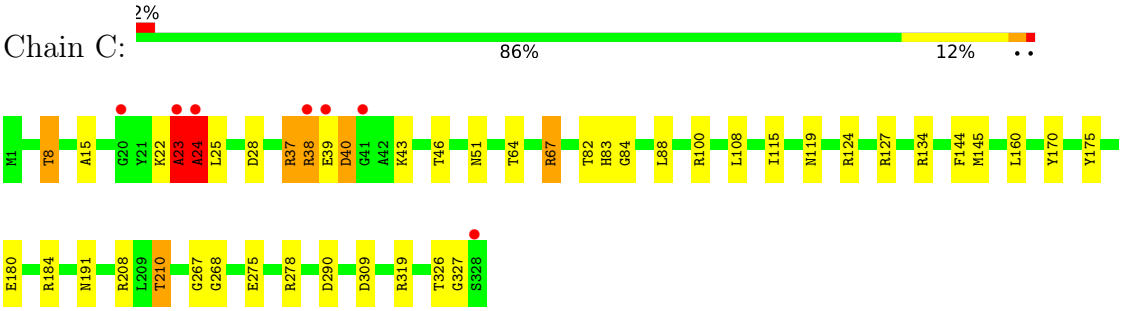
- Molecule 1: L-asparaginase

Chain B:



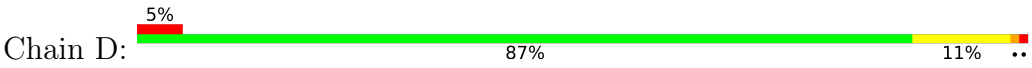
- Molecule 1: L-asparaginase

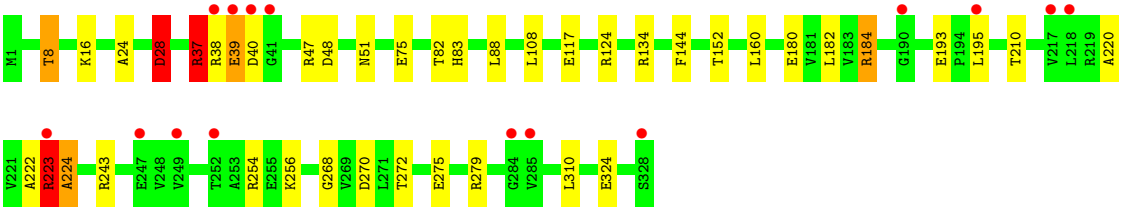
Chain C:



- Molecule 1: L-asparaginase

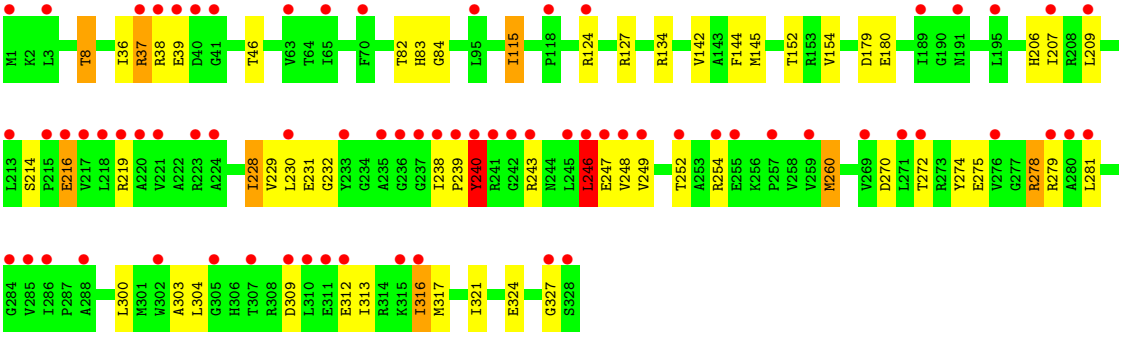
Chain D:





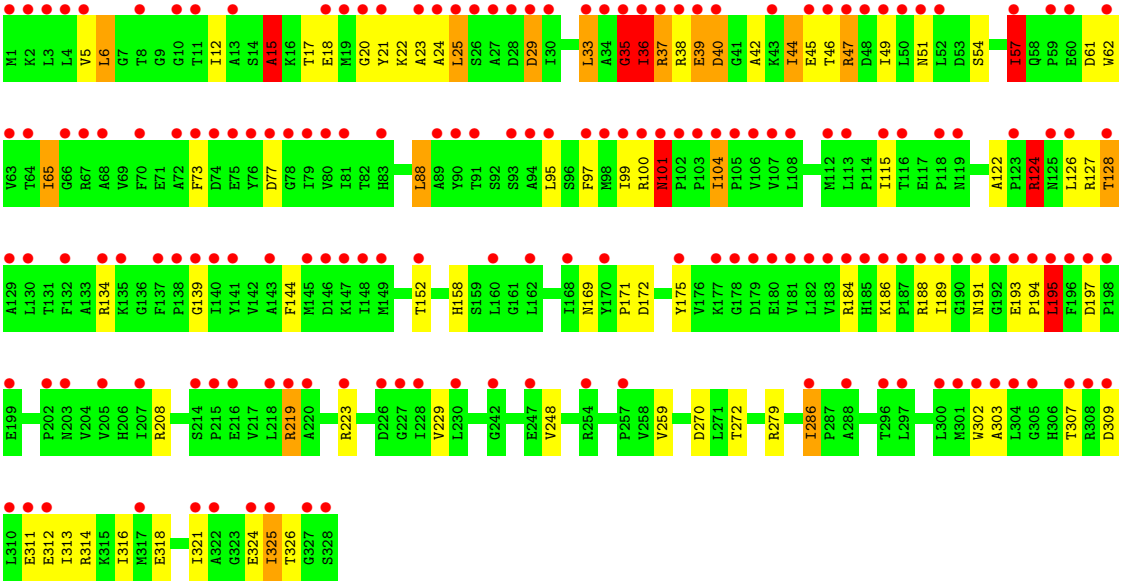
• Molecule 1: L-asparaginase

Chain E:



• Molecule 1: L-asparaginase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	70.74Å 70.96Å 107.73Å 72.13° 76.22° 87.83°	Depositor
Resolution (Å)	68.65 – 2.18 68.65 – 2.18	Depositor EDS
% Data completeness (in resolution range)	97.5 (68.65-2.18) 97.5 (68.65-2.18)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.70 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.194 , 0.224 0.198 , 0.228	Depositor DCC
R_{free} test set	4896 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	49.6	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 61.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h,k,k-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15386	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 4.20% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, PG4, EDO

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	1.06	5/2573 (0.2%)	1.06	13/3491 (0.4%)
1	B	1.01	3/2581 (0.1%)	1.08	16/3503 (0.5%)
1	C	1.05	2/2582 (0.1%)	1.09	10/3503 (0.3%)
1	D	0.98	0/2557	1.09	13/3470 (0.4%)
1	E	0.87	0/2551	1.03	8/3462 (0.2%)
1	F	0.86	1/2562 (0.0%)	1.11	17/3477 (0.5%)
All	All	0.98	11/15406 (0.1%)	1.08	77/20906 (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	B	0	1
1	C	0	2
1	D	0	1
1	E	0	1
1	F	0	2
All	All	0	7

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	170	TYR	CE1-CZ	9.69	1.51	1.38
1	B	141	TYR	CG-CD2	6.17	1.47	1.39
1	B	241	ARG	CZ-NH1	6.16	1.41	1.33
1	A	170	TYR	CE1-CZ	5.92	1.46	1.38
1	A	180	GLU	CD-OE2	5.89	1.32	1.25
1	A	16	LYS	C-O	-5.81	1.12	1.23
1	C	267	GLY	N-CA	-5.63	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	84	GLY	CA-C	5.59	1.60	1.51
1	A	180	GLU	CD-OE1	5.42	1.31	1.25
1	B	29	ASP	CB-CG	5.37	1.63	1.51
1	F	35	GLY	CA-C	5.14	1.60	1.51

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	77	ASP	CB-CG-OD1	12.82	129.84	118.30
1	E	246	LEU	CB-CG-CD2	11.84	131.12	111.00
1	A	124	ARG	NE-CZ-NH2	-9.01	115.80	120.30
1	A	145	MET	CG-SD-CE	8.59	113.94	100.20
1	F	124	ARG	NE-CZ-NH1	7.99	124.30	120.30
1	D	223	ARG	N-CA-C	-7.81	89.92	111.00
1	F	77	ASP	CB-CG-OD2	-7.49	111.56	118.30
1	C	208	ARG	NE-CZ-NH2	-7.39	116.60	120.30
1	F	279	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	D	28	ASP	CB-CG-OD1	7.21	124.79	118.30
1	E	124	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	F	36	ILE	CB-CA-C	7.02	125.65	111.60
1	F	33	LEU	CB-CG-CD2	6.91	122.74	111.00
1	C	23	ALA	CB-CA-C	6.83	120.35	110.10
1	A	134	ARG	CG-CD-NE	-6.81	97.49	111.80
1	B	124	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	F	128	THR	CB-CA-C	6.63	129.50	111.60
1	B	208	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	D	124	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	D	48	ASP	CB-CG-OD1	6.53	124.18	118.30
1	C	67	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	D	224	ALA	N-CA-CB	6.50	119.20	110.10
1	B	28	ASP	CB-CG-OD1	6.46	124.12	118.30
1	F	29	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	F	195	LEU	CA-CB-CG	6.35	129.90	115.30
1	A	67	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	B	48	ASP	CB-CG-OD1	6.26	123.93	118.30
1	C	127	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	A	100	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	F	101	ASN	CB-CG-OD1	-6.20	109.21	121.60
1	B	177	LYS	CD-CE-NZ	6.15	125.84	111.70
1	F	57	ILE	CB-CG1-CD1	6.10	130.98	113.90
1	D	124	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	D	275	GLU	OE1-CD-OE2	-6.02	116.08	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	47	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	F	124	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	F	99	ILE	CB-CG1-CD1	5.89	130.40	113.90
1	B	41	GLY	N-CA-C	-5.86	98.44	113.10
1	D	310	LEU	CB-CG-CD1	5.86	120.96	111.00
1	C	100	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	B	127	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	B	60	GLU	OE1-CD-OE2	-5.77	116.38	123.30
1	A	241	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	C	124	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	E	240	TYR	CA-CB-CG	5.69	124.20	113.40
1	D	24	ALA	N-CA-C	-5.63	95.81	111.00
1	B	124	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	C	327	GLY	N-CA-C	-5.60	99.10	113.10
1	A	124	ARG	CG-CD-NE	-5.58	100.08	111.80
1	F	15	ALA	CB-CA-C	5.58	118.47	110.10
1	A	208	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	B	75	GLU	OE1-CD-OE2	-5.50	116.70	123.30
1	D	48	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	D	117	GLU	OE1-CD-OE2	-5.48	116.73	123.30
1	E	240	TYR	CB-CG-CD1	5.47	124.28	121.00
1	B	195	LEU	CB-CG-CD2	5.42	120.22	111.00
1	B	279	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	E	216	GLU	CA-CB-CG	5.39	125.26	113.40
1	E	127	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	A	241	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	F	25	LEU	CB-CG-CD1	5.33	120.06	111.00
1	B	100	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	226	ASP	CB-CG-OD1	5.26	123.04	118.30
1	F	208	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	C	28	ASP	CB-CG-OD1	5.23	123.01	118.30
1	F	223	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	278	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	C	309	ASP	CB-CG-OD1	5.16	122.94	118.30
1	E	240	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	A	260	MET	CG-SD-CE	-5.10	92.03	100.20
1	A	275	GLU	OE1-CD-OE2	-5.10	117.19	123.30
1	A	195	LEU	CB-CG-CD2	5.09	119.66	111.00
1	D	243	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	C	210	THR	CA-CB-CG2	5.08	119.51	112.40
1	E	246	LEU	CA-CB-CG	5.07	126.95	115.30
1	B	47	ARG	NE-CZ-NH1	5.03	122.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	29	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	40	ASP	Peptide
1	C	24	ALA	Peptide
1	C	326	THR	Peptide
1	D	37	ARG	Peptide
1	E	309	ASP	Mainchain
1	F	35	GLY	Peptide
1	F	39	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	2520	0	2577	28	0
1	B	2523	0	2580	25	1
1	C	2525	0	2581	18	0
1	D	2510	0	2566	16	1
1	E	2507	0	2561	57	0
1	F	2514	0	2568	90	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
2	E	5	0	0	1	0
2	F	5	0	0	0	0
3	A	4	0	6	0	0
3	B	8	0	12	0	0
3	D	8	0	12	1	0
3	F	4	0	6	1	0
4	B	10	0	13	2	0
5	A	55	0	0	1	0
5	B	49	0	0	2	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	35	0	0	1	0
5	D	46	0	0	0	1
5	E	25	0	0	2	0
5	F	13	0	0	2	0
All	All	15386	0	15482	233	2

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 8.

All (233) 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:C:15:ALA:HB2	1:C:25:LEU:HD11	1.30	1.08
1:F:101:ASN:OD1	1:F:194:PRO:HA	1.61	1.00
1:F:65:ILE:HD11	1:F:95:LEU:HD21	1.45	0.98
1:F:24:ALA:HA	1:F:51:ASN:HD21	1.30	0.97
1:F:12:ILE:HD11	1:F:126:LEU:HD21	1.47	0.94
1:F:62:TRP:O	1:F:65:ILE:HD13	1.69	0.93
1:E:274:TYR:O	1:E:278:ARG:HD3	1.71	0.90
1:F:122:ALA:O	1:F:126:LEU:HD23	1.73	0.89
1:B:166:GLN:HG3	5:B:501:HOH:O	1.70	0.89
1:E:240:TYR:CE1	1:E:246:LEU:HB2	2.07	0.88
1:F:15:ALA:HB3	1:F:20:GLY:O	1.74	0.88
1:F:54:SER:HA	1:F:57:ILE:HD13	1.54	0.87
1:F:172:ASP:O	1:F:184:ARG:HD3	1.75	0.86
1:F:25:LEU:HB3	1:F:29:ASP:OD1	1.78	0.83
1:F:62:TRP:HA	1:F:65:ILE:HD12	1.61	0.83
1:F:97:PHE:O	1:F:100:ARG:NH1	2.12	0.81
1:F:65:ILE:CD1	1:F:95:LEU:HD21	2.11	0.80
1:F:23:ALA:O	1:F:51:ASN:ND2	2.15	0.80
1:E:240:TYR:CE2	1:E:246:LEU:HG	2.16	0.80
1:A:307:THR:HG22	1:A:309:ASP:H	1.46	0.80
1:C:15:ALA:HB2	1:C:25:LEU:CD1	2.08	0.80
1:E:313:ILE:O	1:E:316:ILE:HD13	1.82	0.80
1:A:6:LEU:HD22	1:A:49:ILE:HD11	1.63	0.79
1:E:240:TYR:OH	1:E:279:ARG:CB	2.31	0.79
1:F:303:ALA:HB1	1:F:316:ILE:HD11	1.65	0.78
1:B:275:GLU:HG2	1:B:279:ARG:NH1	1.99	0.78
1:F:229:VAL:HG22	1:F:259:VAL:CG1	2.14	0.78
1:F:62:TRP:HA	1:F:65:ILE:CD1	2.15	0.77
1:E:312:GLU:O	1:E:316:ILE:HG23	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:246:LEU:HD13	1:E:247:GLU:N	2.01	0.76
1:F:188:ARG:O	1:F:189:ILE:HG13	1.87	0.75
1:F:101:ASN:HD21	1:F:194:PRO:CD	2.02	0.73
1:A:237:GLY:H	1:A:260:MET:HE1	1.52	0.73
1:C:23:ALA:O	1:C:24:ALA:HB3	1.86	0.73
1:E:206:HIS:CE1	1:E:231:GLU:OE1	2.41	0.73
1:F:219:ARG:HD2	1:F:248:VAL:HG13	1.69	0.73
1:F:35:GLY:O	1:F:36:ILE:HG13	1.88	0.73
1:A:6:LEU:HD22	1:A:49:ILE:CD1	2.19	0.72
1:F:101:ASN:HD21	1:F:194:PRO:N	1.87	0.72
1:F:101:ASN:OD1	1:F:194:PRO:CA	2.38	0.71
1:E:232:GLY:HA3	1:E:260:MET:CE	2.20	0.71
1:F:101:ASN:O	1:F:101:ASN:ND2	2.23	0.71
1:E:240:TYR:OH	1:E:279:ARG:HB3	1.90	0.71
1:F:101:ASN:O	1:F:101:ASN:CG	2.29	0.71
1:F:219:ARG:CD	1:F:248:VAL:HG13	2.21	0.70
1:E:303:ALA:HB2	1:E:316:ILE:HD11	1.72	0.70
1:E:8:THR:HG22	1:E:83:HIS:HA	1.76	0.68
1:A:237:GLY:H	1:A:260:MET:CE	2.06	0.67
1:C:8:THR:HG22	1:C:83:HIS:HA	1.76	0.67
1:E:240:TYR:OH	1:E:279:ARG:HB2	1.95	0.66
1:F:307:THR:HG21	1:F:312:GLU:HG3	1.76	0.66
1:F:259:VAL:HG23	1:F:286:ILE:HG23	1.77	0.66
1:D:8:THR:HG22	1:D:83:HIS:HA	1.78	0.65
1:F:24:ALA:HA	1:F:51:ASN:ND2	2.08	0.65
1:B:8:THR:HG22	1:B:83:HIS:HA	1.79	0.64
1:F:100:ARG:O	1:F:101:ASN:OD1	2.15	0.64
1:A:32:GLN:NE2	1:D:182:LEU:HD13	2.14	0.62
1:C:37:ARG:O	1:C:39:GLU:N	2.33	0.62
1:E:228:ILE:HD11	1:E:230:LEU:HD23	1.81	0.61
1:F:37:ARG:O	1:F:39:GLU:N	2.34	0.61
1:F:158[A]:HIS:CE1	5:F:504:HOH:O	2.52	0.61
1:A:236:GLY:CA	1:A:260:MET:HE2	2.31	0.61
1:A:236:GLY:HA2	1:A:260:MET:CE	2.31	0.61
1:F:172:ASP:O	1:F:184:ARG:CD	2.49	0.61
1:F:101:ASN:ND2	1:F:194:PRO:N	2.49	0.60
1:B:34:ALA:CB	1:B:36:ILE:HD13	2.31	0.60
1:F:101:ASN:OD1	1:F:193:GLU:O	2.18	0.60
1:A:37:ARG:O	1:A:39:GLU:N	2.33	0.60
1:E:37:ARG:O	1:E:39:GLU:N	2.33	0.60
1:E:303:ALA:CB	1:E:316:ILE:HD11	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:ARG:O	1:B:39:GLU:N	2.34	0.60
1:F:61:ASP:O	1:F:65:ILE:HG23	2.01	0.60
1:C:23:ALA:O	1:C:24:ALA:CB	2.50	0.60
1:F:309:ASP:HB3	1:F:312:GLU:CD	2.22	0.59
1:B:124:ARG:NH1	1:B:127:ARG:HH11	2.01	0.58
1:F:35:GLY:O	1:F:36:ILE:CG1	2.50	0.58
1:B:16:LYS:HE3	1:B:20:GLY:HA2	1.86	0.58
1:B:83:HIS:HD2	1:B:84:GLY:O	1.87	0.58
1:D:37:ARG:O	1:D:39:GLU:N	2.37	0.58
1:F:229:VAL:HG22	1:F:259:VAL:HG11	1.84	0.58
1:E:274:TYR:O	1:E:278:ARG:CD	2.47	0.58
1:E:209:LEU:HD11	1:E:238:ILE:CD1	2.34	0.57
1:D:220:ALA:O	1:D:223:ARG:O	2.22	0.57
1:F:259:VAL:HA	1:F:286:ILE:HG22	1.86	0.57
1:F:172:ASP:HB2	1:F:184:ARG:HD2	1.87	0.56
1:E:240:TYR:CD1	1:E:246:LEU:CB	2.89	0.56
1:F:39:GLU:O	1:F:40:ASP:CG	2.44	0.55
1:F:313:ILE:O	1:F:316:ILE:HG12	2.06	0.55
1:F:325:ILE:HD13	1:F:326:THR:O	2.07	0.55
1:E:313:ILE:O	1:E:316:ILE:CD1	2.55	0.55
1:F:65:ILE:HD11	1:F:95:LEU:CD2	2.26	0.55
1:A:270:ASP:OD1	1:A:272:THR:HB	2.07	0.54
1:E:232:GLY:HA3	1:E:260:MET:HE2	1.89	0.54
1:F:15:ALA:CB	1:F:20:GLY:O	2.51	0.54
1:C:24:ALA:HB2	1:C:51:ASN:HD21	1.72	0.54
1:E:240:TYR:CD1	1:E:246:LEU:HB3	2.42	0.54
1:B:46:THR:OG1	4:B:404:PG4:H41	2.08	0.54
1:E:240:TYR:CZ	1:E:246:LEU:HB2	2.43	0.54
1:F:6:LEU:HD13	1:F:47:ARG:HB3	1.89	0.54
1:E:270:ASP:OD1	1:E:272:THR:HB	2.08	0.53
1:F:270:ASP:OD1	1:F:272:THR:HB	2.07	0.53
1:B:270:ASP:OD1	1:B:272:THR:HB	2.08	0.53
1:A:236:GLY:CA	1:A:260:MET:CE	2.86	0.53
1:D:270:ASP:OD1	1:D:272:THR:HB	2.08	0.53
1:E:316:ILE:HD13	1:E:317:MET:N	2.23	0.53
1:F:6:LEU:HD11	1:F:49:ILE:HG13	1.89	0.53
1:E:249:VAL:HA	1:E:252:THR:HG22	1.89	0.53
1:E:238:ILE:O	1:E:240:TYR:CD1	2.61	0.53
1:F:286:ILE:HD11	1:F:318:GLU:HG3	1.91	0.53
1:E:84:GLY:HA3	2:E:401:PO4:O4	2.09	0.52
1:E:214:SER:OG	1:E:216:GLU:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:17:THR:HA	1:F:21:TYR:CE2	2.45	0.52
1:F:5:VAL:HG23	1:F:44:ILE:HD11	1.91	0.52
1:C:22:LYS:C	1:C:23:ALA:O	2.48	0.52
1:E:300:LEU:O	1:E:304:LEU:HD23	2.10	0.52
1:B:34:ALA:HB3	1:B:36:ILE:HD13	1.92	0.51
1:E:313:ILE:HA	1:E:316:ILE:HD12	1.91	0.51
1:E:8:THR:CG2	1:E:83:HIS:HA	2.41	0.51
1:B:124:ARG:NH1	1:B:127:ARG:NH1	2.57	0.51
1:C:275:GLU:HG3	1:C:278:ARG:NH2	2.26	0.51
1:E:115:ILE:HG22	5:E:511:HOH:O	2.11	0.51
1:A:248:VAL:O	1:A:251:GLU:HG2	2.11	0.50
1:F:12:ILE:CD1	1:F:126:LEU:HD21	2.31	0.50
1:F:17:THR:HG23	1:F:18:GLU:OE1	2.12	0.50
1:E:316:ILE:HD13	1:E:317:MET:H	1.77	0.50
1:F:88:LEU:HD23	1:F:88:LEU:O	2.11	0.50
1:E:240:TYR:CZ	1:E:246:LEU:HG	2.47	0.50
1:F:219:ARG:HD3	1:F:248:VAL:HG22	1.94	0.50
1:E:206:HIS:HE1	1:E:231:GLU:OE1	1.93	0.49
1:F:5:VAL:CG2	1:F:44:ILE:HD11	2.42	0.49
1:F:309:ASP:HB3	1:F:312:GLU:HG2	1.93	0.49
1:F:313:ILE:HA	1:F:316:ILE:CD1	2.42	0.49
1:A:36:ILE:HG22	1:A:37:ARG:N	2.27	0.49
1:A:237:GLY:N	1:A:260:MET:HE2	2.28	0.49
1:B:48:ASP:OD2	4:B:404:PG4:H62	2.13	0.49
1:E:240:TYR:CD2	1:E:246:LEU:HG	2.48	0.49
1:F:313:ILE:HA	1:F:316:ILE:HD11	1.95	0.49
1:A:237:GLY:N	1:A:260:MET:CE	2.73	0.48
1:B:275:GLU:CG	1:B:279:ARG:NH1	2.72	0.48
1:B:34:ALA:HB1	1:B:36:ILE:HD13	1.95	0.48
1:C:8:THR:CG2	1:C:83:HIS:HA	2.42	0.48
1:F:101:ASN:HD21	1:F:194:PRO:CG	2.27	0.48
1:E:240:TYR:CD1	1:E:246:LEU:HB2	2.46	0.48
1:F:40:ASP:OD1	1:F:42:ALA:O	2.31	0.48
1:E:249:VAL:HA	1:E:252:THR:CG2	2.44	0.48
1:F:35:GLY:C	1:F:36:ILE:HG13	2.34	0.47
1:F:127:ARG:HG3	1:F:128:THR:HG23	1.96	0.47
1:F:44:ILE:HG23	1:F:44:ILE:O	2.14	0.47
1:D:254:ARG:HB3	1:D:254:ARG:NH1	2.28	0.47
1:A:270:ASP:HB3	1:A:273:ARG:HD3	1.97	0.47
1:D:8:THR:CG2	1:D:83:HIS:HA	2.44	0.47
1:F:23:ALA:O	1:F:51:ASN:CG	2.52	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:309:ASP:HB3	1:F:312:GLU:CG	2.44	0.47
1:B:314:ARG:NH1	1:B:318:GLU:OE1	2.48	0.47
1:F:259:VAL:HA	1:F:286:ILE:CG2	2.45	0.47
1:E:303:ALA:HB2	1:E:316:ILE:CD1	2.43	0.46
1:F:171:PRO:CB	1:F:184:ARG:HE	2.28	0.46
1:F:158[A]:HIS:HE1	5:F:504:HOH:O	1.94	0.46
1:A:121:ASP:HB2	1:A:124:ARG:NH2	2.30	0.46
1:A:84:GLY:HA3	2:A:401:PO4:O1	2.16	0.46
1:F:122:ALA:O	1:F:126:LEU:CD2	2.54	0.45
1:B:124:ARG:HA	1:B:127:ARG:NH1	2.31	0.45
1:F:100:ARG:NH2	1:F:302:TRP:CH2	2.83	0.45
1:A:327:GLY:O	1:A:328:SER:C	2.54	0.45
1:B:8:THR:HG23	5:B:532:HOH:O	2.17	0.45
1:E:206:HIS:NE2	1:E:231:GLU:OE1	2.48	0.45
1:E:238:ILE:O	1:E:240:TYR:CE1	2.70	0.45
1:E:275:GLU:CD	1:E:275:GLU:H	2.20	0.45
1:F:44:ILE:C	1:F:44:ILE:HD13	2.37	0.45
1:F:44:ILE:HD13	1:F:45:GLU:N	2.32	0.45
1:B:182:LEU:N	1:B:182:LEU:HD12	2.32	0.44
1:E:240:TYR:CE1	1:E:246:LEU:CB	2.87	0.44
1:F:303:ALA:HB1	1:F:316:ILE:CD1	2.39	0.44
1:C:22:LYS:O	1:C:23:ALA:O	2.34	0.44
1:E:228:ILE:CD1	1:E:230:LEU:CD2	2.96	0.44
1:B:37:ARG:NH1	1:B:42:ALA:O	2.50	0.44
1:F:169:ASN:HD21	3:F:402:EDO:C1	2.30	0.44
1:D:8:THR:HG22	1:D:82:THR:O	2.17	0.44
1:F:62:TRP:C	1:F:65:ILE:HD13	2.34	0.44
1:E:8:THR:HG22	1:E:82:THR:O	2.18	0.44
1:F:152:THR:OG1	1:F:324:GLU:HB3	2.17	0.44
1:F:62:TRP:CA	1:F:65:ILE:CD1	2.93	0.44
1:D:88:LEU:HD11	1:D:108:LEU:HB3	2.00	0.43
1:D:184:ARG:C	1:D:184:ARG:CD	2.86	0.43
1:D:184:ARG:HD3	1:D:184:ARG:O	2.18	0.43
1:D:268:GLY:HA2	3:D:403:EDO:H22	2.00	0.43
1:A:314:ARG:NH1	1:A:318:GLU:OE1	2.51	0.43
1:D:51:ASN:CG	1:D:51:ASN:O	2.56	0.43
1:D:152:THR:OG1	1:D:324:GLU:HB3	2.19	0.43
1:F:73:PHE:HD1	1:F:104:ILE:HD11	1.84	0.43
1:C:84:GLY:HA3	2:C:401:PO4:O4	2.18	0.43
1:E:152:THR:OG1	1:E:324:GLU:HB3	2.18	0.43
1:F:54:SER:HA	1:F:57:ILE:CD1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:ALA:O	1:D:256:LYS:NZ	2.47	0.43
1:A:97:PHE:O	1:A:100:ARG:NH2	2.52	0.43
1:A:232:GLY:HA3	1:A:260:MET:CE	2.49	0.42
1:B:152[A]:THR:OG1	1:B:324:GLU:HB3	2.18	0.42
1:E:248:VAL:O	1:E:252:THR:HG22	2.19	0.42
1:E:303:ALA:CB	1:E:316:ILE:CD1	2.96	0.42
1:A:6:LEU:HD22	1:A:49:ILE:HD12	2.00	0.42
1:B:8:THR:HG22	1:B:82:THR:O	2.19	0.42
1:A:124:ARG:NE	1:A:145:MET:HA	2.34	0.42
1:C:88:LEU:HD11	1:C:108:LEU:HB3	2.02	0.42
1:F:303:ALA:CB	1:F:316:ILE:CD1	2.97	0.42
1:A:222:ALA:O	1:A:256:LYS:NZ	2.46	0.42
1:F:311:GLU:OE1	1:F:314:ARG:NH1	2.50	0.42
1:A:190:GLY:HA2	5:A:549:HOH:O	2.18	0.42
1:E:239:PRO:C	1:E:240:TYR:HD1	2.23	0.42
1:E:272:THR:O	1:E:278:ARG:NH1	2.42	0.42
1:C:8:THR:HG23	5:C:520:HOH:O	2.20	0.41
1:E:8:THR:HG23	5:E:512:HOH:O	2.20	0.41
1:E:240:TYR:CZ	1:E:279:ARG:CB	3.03	0.41
1:B:51:ASN:O	1:B:51:ASN:CG	2.58	0.41
1:C:8:THR:HG22	1:C:82:THR:O	2.20	0.41
1:F:15:ALA:N	1:F:20:GLY:O	2.53	0.41
1:F:139:GLY:HA3	1:F:189:ILE:HD13	2.01	0.41
1:D:184:ARG:CD	1:D:184:ARG:O	2.68	0.41
1:E:142:VAL:HG21	1:E:154:VAL:HG21	2.02	0.41
1:E:240:TYR:CG	1:E:246:LEU:HB3	2.56	0.41
1:F:195:LEU:HD13	1:F:197:ASP:HB2	2.03	0.41
1:F:303:ALA:CB	1:F:316:ILE:HD11	2.45	0.41
1:F:175:TYR:OH	1:F:184:ARG:NH1	2.54	0.41
1:F:124:ARG:HD3	1:F:124:ARG:H	1.85	0.40
1:A:121:ASP:HB2	1:A:124:ARG:HH22	1.86	0.40
1:A:186:LYS:HE2	1:A:189:ILE:HD12	2.04	0.40
1:C:119:ASN:HD22	1:C:119:ASN:HA	1.73	0.40
1:C:175:TYR:OH	1:C:184[B]:ARG:NH1	2.54	0.40
1:E:36:ILE:HG22	1:E:37:ARG:N	2.37	0.40
1:E:228:ILE:HD13	1:E:229:VAL:C	2.41	0.40
1:C:268:GLY:HA3	1:C:290:ASP:HA	2.03	0.40
1:F:124:ARG:O	1:F:127:ARG:HG2	2.22	0.40

All (2) 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)
5:B:504:HOH:O	5:D:502:HOH:O[1_445]	1.05	1.15
1:B:51:ASN:OD1	1:D:28:ASP:OD2[1_445]	2.14	0.06

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	328/328 (100%)	321 (98%)	5 (2%)	2 (1%)	25	24
1	B	330/328 (101%)	319 (97%)	9 (3%)	2 (1%)	25	24
1	C	329/328 (100%)	315 (96%)	9 (3%)	5 (2%)	10	7
1	D	327/328 (100%)	316 (97%)	7 (2%)	4 (1%)	13	9
1	E	326/328 (99%)	315 (97%)	8 (2%)	3 (1%)	17	15
1	F	327/328 (100%)	306 (94%)	14 (4%)	7 (2%)	7	3
All	All	1967/1968 (100%)	1892 (96%)	52 (3%)	23 (1%)	13	9

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	38	ARG
1	B	37	ARG
1	B	38	ARG
1	C	37	ARG
1	C	38	ARG
1	D	37	ARG
1	D	38	ARG
1	D	224	ALA
1	E	37	ARG
1	E	38	ARG
1	F	15	ALA
1	F	36	ILE
1	F	37	ARG

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Mol	Chain	Res	Type
1	F	38	ARG
1	F	40	ASP
1	F	191	ASN
1	C	23	ALA
1	C	24	ALA
1	F	22	LYS
1	C	40	ASP
1	D	40	ASP
1	E	327	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	269/267 (101%)	259 (96%)	10 (4%)	34	40
1	B	271/267 (102%)	259 (96%)	12 (4%)	28	33
1	C	270/267 (101%)	254 (94%)	16 (6%)	19	21
1	D	268/267 (100%)	253 (94%)	15 (6%)	21	23
1	E	267/267 (100%)	247 (92%)	20 (8%)	13	12
1	F	268/267 (100%)	247 (92%)	21 (8%)	12	11
All	All	1613/1602 (101%)	1519 (94%)	94 (6%)	19	21

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	100	ARG
1	A	115	ILE
1	A	144	PHE
1	A	145	MET
1	A	163	ASN
1	A	180	GLU
1	A	195	LEU
1	A	319	ARG

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Mol	Chain	Res	Type
1	A	321	ILE
1	B	8	THR
1	B	28	ASP
1	B	39	GLU
1	B	75	GLU
1	B	124	ARG
1	B	134	ARG
1	B	144	PHE
1	B	180	GLU
1	B	195	LEU
1	B	219	ARG
1	B	275	GLU
1	B	315	LYS
1	C	8	THR
1	C	38	ARG
1	C	40	ASP
1	C	43	LYS
1	C	46	THR
1	C	64	THR
1	C	67	ARG
1	C	115	ILE
1	C	134	ARG
1	C	144	PHE
1	C	145	MET
1	C	160	LEU
1	C	180	GLU
1	C	191	ASN
1	C	210	THR
1	C	319	ARG
1	D	8	THR
1	D	16	LYS
1	D	28	ASP
1	D	39	GLU
1	D	75	GLU
1	D	134	ARG
1	D	144	PHE
1	D	160	LEU
1	D	180	GLU
1	D	184	ARG
1	D	193	GLU
1	D	195	LEU
1	D	210	THR

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Mol	Chain	Res	Type
1	D	223	ARG
1	D	279	ARG
1	E	8	THR
1	E	46	THR
1	E	115	ILE
1	E	134	ARG
1	E	144	PHE
1	E	145	MET
1	E	179	ASP
1	E	180	GLU
1	E	207	ILE
1	E	219	ARG
1	E	228	ILE
1	E	240	TYR
1	E	243	ARG
1	E	246	LEU
1	E	254	ARG
1	E	260	MET
1	E	278	ARG
1	E	281	LEU
1	E	316	ILE
1	E	321	ILE
1	F	6	LEU
1	F	33	LEU
1	F	36	ILE
1	F	44	ILE
1	F	46	THR
1	F	47	ARG
1	F	57	ILE
1	F	65	ILE
1	F	88	LEU
1	F	101	ASN
1	F	104	ILE
1	F	115	ILE
1	F	124	ARG
1	F	134	ARG
1	F	144	PHE
1	F	186	LYS
1	F	195	LEU
1	F	219	ARG
1	F	286	ILE
1	F	321	ILE

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Mol	Chain	Res	Type
1	F	325	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	163	ASN
1	B	83	HIS
1	B	163	ASN
1	B	166	GLN
1	C	119	ASN
1	E	163	ASN
1	F	51	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

13 ligands 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	$\#\|Z\|>2$
2	PO4	C	401	-	4,4,4	1.67	1 (25%)	6,6,6	3.23	5 (83%)
3	EDO	D	402	-	3,3,3	0.51	0	2,2,2	0.84	0
4	PG4	B	404	-	9,9,12	0.44	0	8,8,11	1.07	1 (12%)
3	EDO	B	402	-	3,3,3	0.69	0	2,2,2	0.61	0
3	EDO	D	403	-	3,3,3	0.72	0	2,2,2	0.51	0
3	EDO	F	402	-	3,3,3	0.60	0	2,2,2	0.19	0
2	PO4	A	401	-	4,4,4	2.12	1 (25%)	6,6,6	2.41	2 (33%)
3	EDO	A	402	-	3,3,3	1.10	0	2,2,2	0.48	0
2	PO4	E	401	-	4,4,4	1.92	1 (25%)	6,6,6	1.87	3 (50%)
3	EDO	B	403	-	3,3,3	0.60	0	2,2,2	0.90	0
2	PO4	D	401	-	4,4,4	2.47	2 (50%)	6,6,6	3.93	5 (83%)
2	PO4	F	401	-	4,4,4	2.14	1 (25%)	6,6,6	1.26	1 (16%)
2	PO4	B	401	-	4,4,4	2.11	1 (25%)	6,6,6	3.15	3 (50%)

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
3	EDO	D	402	-	-	1/1/1/1	-
4	PG4	B	404	-	-	5/7/7/10	-
3	EDO	B	402	-	-	0/1/1/1	-
3	EDO	D	403	-	-	1/1/1/1	-
3	EDO	F	402	-	-	1/1/1/1	-
3	EDO	A	402	-	-	0/1/1/1	-
3	EDO	B	403	-	-	1/1/1/1	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	PO4	P-O4	-3.89	1.42	1.54
2	F	401	PO4	P-O1	3.87	1.59	1.50
2	A	401	PO4	P-O2	-3.47	1.44	1.54
2	B	401	PO4	P-O4	-2.94	1.45	1.54
2	D	401	PO4	P-O2	-2.89	1.45	1.54
2	C	401	PO4	P-O3	-2.83	1.46	1.54
2	E	401	PO4	P-O4	-2.81	1.46	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	PO4	O4-P-O1	-6.00	88.92	110.89
2	B	401	PO4	O2-P-O1	-5.71	90.00	110.89
2	C	401	PO4	O4-P-O3	5.08	124.26	107.97
2	D	401	PO4	O3-P-O2	-4.53	93.43	107.97
2	B	401	PO4	O3-P-O2	3.92	120.56	107.97
2	D	401	PO4	O4-P-O3	3.90	120.50	107.97
2	A	401	PO4	O2-P-O1	3.82	124.86	110.89
2	A	401	PO4	O4-P-O2	-3.57	96.51	107.97
2	C	401	PO4	O3-P-O1	-3.40	98.44	110.89
2	D	401	PO4	O2-P-O1	3.39	123.29	110.89
2	C	401	PO4	O3-P-O2	3.37	118.79	107.97
2	B	401	PO4	O4-P-O2	3.23	118.35	107.97
2	C	401	PO4	O4-P-O2	-3.11	98.00	107.97
2	E	401	PO4	O4-P-O3	2.69	116.61	107.97
2	E	401	PO4	O4-P-O1	-2.56	101.54	110.89
2	D	401	PO4	O4-P-O2	2.52	116.05	107.97
2	F	401	PO4	O3-P-O2	2.38	115.60	107.97
2	E	401	PO4	O3-P-O2	-2.24	100.77	107.97
4	B	404	PG4	O1-C1-C2	-2.07	99.78	111.81
2	C	401	PO4	O2-P-O1	-2.03	103.46	110.89

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	404	PG4	O2-C3-C4-O3
4	B	404	PG4	O1-C1-C2-O2
4	B	404	PG4	C6-C5-O3-C4
3	F	402	EDO	O1-C1-C2-O2
4	B	404	PG4	C1-C2-O2-C3
4	B	404	PG4	O3-C5-C6-O4
3	B	403	EDO	O1-C1-C2-O2
3	D	403	EDO	O1-C1-C2-O2
3	D	402	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	PO4	1	0
4	B	404	PG4	2	0
3	D	403	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	402	EDO	1	0
2	A	401	PO4	1	0
2	E	401	PO4	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	328/328 (100%)	0.45	7 (2%) 63 64	34, 56, 96, 147	0
1	B	328/328 (100%)	0.49	5 (1%) 73 74	41, 64, 107, 150	0
1	C	328/328 (100%)	0.53	7 (2%) 63 64	36, 61, 105, 145	0
1	D	328/328 (100%)	0.61	15 (4%) 32 33	41, 64, 106, 165	0
1	E	328/328 (100%)	1.23	71 (21%) 0 0	44, 78, 146, 180	0
1	F	328/328 (100%)	2.57	174 (53%) 0 0	56, 115, 167, 205	0
All	All	1968/1968 (100%)	0.98	279 (14%) 2 2	34, 69, 140, 205	0

All (279) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	328	SER	13.1
1	F	78	GLY	12.3
1	E	328	SER	11.9
1	E	240	TYR	11.8
1	E	242	GLY	11.7
1	F	49	ILE	10.9
1	F	106	VAL	10.7
1	F	24	ALA	10.2
1	F	178	GLY	10.2
1	E	327	GLY	9.4
1	F	104	ILE	9.1
1	E	238	ILE	8.9
1	E	254	ARG	8.8
1	D	38	ARG	8.7
1	F	74	ASP	8.7
1	E	316	ILE	8.5
1	F	21	TYR	8.2
1	F	70	PHE	8.0
1	E	284	GLY	7.8

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Mol	Chain	Res	Type	RSRZ
1	F	95	LEU	7.4
1	E	38	ARG	7.2
1	F	134	ARG	7.2
1	F	139	GLY	7.0
1	E	271	LEU	6.9
1	F	183	VAL	6.9
1	E	39	GLU	6.7
1	F	305	GLY	6.7
1	F	130	LEU	6.7
1	F	20	GLY	6.7
1	F	322	ALA	6.6
1	F	33	LEU	6.6
1	F	189	ILE	6.6
1	F	4	LEU	6.5
1	F	182	LEU	6.3
1	F	68	ALA	6.3
1	E	248	VAL	6.2
1	B	38	ARG	6.2
1	F	23	ALA	6.2
1	F	39	GLU	6.1
1	F	19	MET	6.1
1	F	30	ILE	6.0
1	F	132	PHE	5.9
1	F	162	LEU	5.9
1	F	300	LEU	5.8
1	F	45	GLU	5.8
1	F	175	TYR	5.7
1	D	41	GLY	5.7
1	E	219	ARG	5.7
1	F	102	PRO	5.6
1	F	126	LEU	5.5
1	F	219	ARG	5.5
1	F	46	THR	5.5
1	D	39	GLU	5.5
1	F	76	TYR	5.4
1	F	115	ILE	5.4
1	C	24	ALA	5.4
1	F	180	GLU	5.4
1	F	149	MET	5.3
1	F	37	ARG	5.3
1	C	20	GLY	5.2
1	F	296	THR	5.2

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Mol	Chain	Res	Type	RSRZ
1	F	190	GLY	5.2
1	F	227	GLY	5.2
1	F	108	LEU	5.2
1	F	193	GLU	5.2
1	F	179	ASP	5.1
1	E	286	ILE	5.1
1	F	205	VAL	5.1
1	E	259	VAL	5.1
1	F	59	PRO	5.1
1	F	25	LEU	5.1
1	C	328	SER	5.0
1	E	209	LEU	5.0
1	F	50	LEU	5.0
1	F	143	ALA	4.9
1	E	281	LEU	4.8
1	E	220	ALA	4.8
1	F	5	VAL	4.8
1	F	207	ILE	4.8
1	D	328	SER	4.8
1	E	195	LEU	4.7
1	E	224	ALA	4.7
1	E	223	ARG	4.7
1	F	83	HIS	4.7
1	F	40	ASP	4.7
1	F	79	ILE	4.5
1	E	191	ASN	4.5
1	E	285	VAL	4.4
1	F	38	ARG	4.4
1	C	38	ARG	4.4
1	F	254	ARG	4.4
1	A	40	ASP	4.4
1	F	75	GLU	4.3
1	F	73	PHE	4.3
1	F	18	GLU	4.3
1	F	11	THR	4.3
1	F	257	PRO	4.3
1	F	34	ALA	4.2
1	C	23	ALA	4.1
1	F	63	VAL	4.1
1	A	191	ASN	4.1
1	F	317	MET	4.1
1	F	93	SER	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	113	LEU	4.0
1	F	51	ASN	4.0
1	F	145	MET	4.0
1	C	39	GLU	3.9
1	E	236	GLY	3.8
1	F	47	ARG	3.8
1	E	217	VAL	3.8
1	F	107	VAL	3.8
1	D	223	ARG	3.8
1	F	223	ARG	3.8
1	B	182	LEU	3.7
1	F	52	LEU	3.7
1	F	197	ASP	3.7
1	F	94	ALA	3.7
1	F	100	ARG	3.7
1	F	138	PRO	3.7
1	F	312	GLU	3.7
1	E	272	THR	3.7
1	E	309	ASP	3.6
1	F	192	GLY	3.6
1	F	327	GLY	3.6
1	F	170	TYR	3.6
1	F	97	PHE	3.6
1	F	72	ALA	3.6
1	F	77	ASP	3.6
1	F	148	ILE	3.5
1	F	103	PRO	3.5
1	A	190	GLY	3.5
1	F	168	ILE	3.5
1	F	325	ILE	3.5
1	F	160	LEU	3.4
1	F	105	PRO	3.4
1	E	213	LEU	3.4
1	E	221	VAL	3.4
1	F	27	ALA	3.3
1	F	188	ARG	3.3
1	E	311	GLU	3.3
1	D	195	LEU	3.3
1	F	90	TYR	3.3
1	F	304	LEU	3.3
1	F	302	TRP	3.2
1	F	195	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	F	152	THR	3.2
1	B	328	SER	3.2
1	F	13	ALA	3.2
1	E	246	LEU	3.2
1	E	252	THR	3.1
1	F	309	ASP	3.1
1	A	328	SER	3.1
1	F	62	TRP	3.1
1	E	257	PRO	3.1
1	E	218	LEU	3.1
1	F	214	SER	3.1
1	F	43	LYS	3.1
1	F	242	GLY	3.1
1	E	243	ARG	3.1
1	E	235	ALA	3.1
1	F	129	ALA	3.1
1	F	1	MET	3.1
1	F	98	MET	3.1
1	F	286	ILE	3.1
1	D	284	GLY	3.0
1	E	280	ALA	3.0
1	F	36	ILE	3.0
1	D	218	LEU	3.0
1	F	297	LEU	3.0
1	E	302	TRP	3.0
1	F	81	ILE	3.0
1	F	8	THR	3.0
1	F	35	GLY	3.0
1	F	186	LYS	3.0
1	E	230	LEU	2.9
1	F	3	LEU	2.9
1	F	67	ARG	2.9
1	F	324	GLU	2.9
1	F	199	GLU	2.9
1	F	135	LYS	2.8
1	F	194	PRO	2.8
1	F	218	LEU	2.8
1	F	226	ASP	2.8
1	F	137	PHE	2.8
1	E	215	PRO	2.8
1	D	40	ASP	2.8
1	E	315	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	288	ALA	2.7
1	F	181	VAL	2.7
1	E	276	VAL	2.7
1	F	184	ARG	2.7
1	F	196	PHE	2.7
1	F	26	SER	2.7
1	A	39	GLU	2.7
1	E	255	GLU	2.7
1	D	252	THR	2.7
1	E	247	GLU	2.7
1	E	245	LEU	2.7
1	F	60	GLU	2.7
1	E	95	LEU	2.7
1	D	249	VAL	2.7
1	E	312	GLU	2.7
1	F	118	PRO	2.7
1	F	310	LEU	2.6
1	E	216	GLU	2.6
1	F	191	ASN	2.6
1	F	99	ILE	2.6
1	F	64	THR	2.6
1	F	128	THR	2.6
1	F	48	ASP	2.6
1	B	100	ARG	2.5
1	F	28	ASP	2.5
1	F	230	LEU	2.5
1	F	216	GLU	2.5
1	E	249	VAL	2.5
1	F	116	THR	2.5
1	E	239	PRO	2.5
1	D	217	VAL	2.5
1	F	123	PRO	2.5
1	F	125	ASN	2.4
1	F	177	LYS	2.4
1	F	203	ASN	2.4
1	E	269	VAL	2.4
1	E	279	ARG	2.4
1	F	140	ILE	2.4
1	F	66	GLY	2.4
1	F	308	ARG	2.4
1	F	198	PRO	2.4
1	F	228	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	285	VAL	2.3
1	E	65	ILE	2.3
1	F	185	HIS	2.3
1	F	89	ALA	2.3
1	B	1	MET	2.3
1	F	321	ILE	2.3
1	F	147	LYS	2.3
1	E	124	ARG	2.3
1	F	57	ILE	2.3
1	F	119	ASN	2.3
1	F	303	ALA	2.2
1	F	141	TYR	2.2
1	F	247	GLU	2.2
1	E	37	ARG	2.2
1	E	288	ALA	2.2
1	F	101	ASN	2.2
1	A	38	ARG	2.2
1	E	3	LEU	2.2
1	E	118	PRO	2.2
1	E	40	ASP	2.2
1	D	190	GLY	2.2
1	E	63	VAL	2.2
1	D	247	GLU	2.2
1	E	41	GLY	2.2
1	E	307	THR	2.2
1	E	70	PHE	2.1
1	E	233	TYR	2.1
1	F	220	ALA	2.1
1	F	29	ASP	2.1
1	F	215	PRO	2.1
1	F	2	LYS	2.1
1	E	241	ARG	2.1
1	E	1	MET	2.1
1	F	112	MET	2.1
1	F	80	VAL	2.1
1	A	41	GLY	2.1
1	F	91	THR	2.0
1	C	41	GLY	2.0
1	E	237	GLY	2.0
1	E	305	GLY	2.0
1	F	10	GLY	2.0
1	F	146	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	187	PRO	2.0
1	F	202	PRO	2.0
1	E	189	ILE	2.0
1	E	207	ILE	2.0
1	E	310	LEU	2.0
1	F	301	MET	2.0
1	F	311	GLU	2.0
1	F	307	THR	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	PO4	F	401	5/5	0.88	0.16	98,99,103,106	0
4	PG4	B	404	10/13	0.89	0.20	73,79,89,90	0
3	EDO	B	403	4/4	0.93	0.21	60,61,66,66	0
3	EDO	A	402	4/4	0.95	0.16	42,43,44,45	0
3	EDO	F	402	4/4	0.95	0.16	68,72,72,75	0
3	EDO	B	402	4/4	0.95	0.17	48,51,52,53	0
3	EDO	D	402	4/4	0.96	0.20	59,60,63,65	0
2	PO4	C	401	5/5	0.98	0.16	62,63,69,71	0
3	EDO	D	403	4/4	0.98	0.14	58,61,62,65	0
2	PO4	E	401	5/5	0.99	0.12	50,53,54,55	0
2	PO4	A	401	5/5	0.99	0.19	41,45,48,48	0
2	PO4	D	401	5/5	0.99	0.16	46,48,55,56	0
2	PO4	B	401	5/5	1.00	0.19	49,49,54,57	0

6.5 Other polymers (i)

There are no such residues in this entry.