



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2026 – 12:10 AM UTC

PDB ID : 5LU0 / pdb_00005lu0
Title : Crystal structure of H. pylori referent strain in complex with PO4
Authors : Stefanic, Z.
Deposited on : 2016-09-07
Resolution : 1.73 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

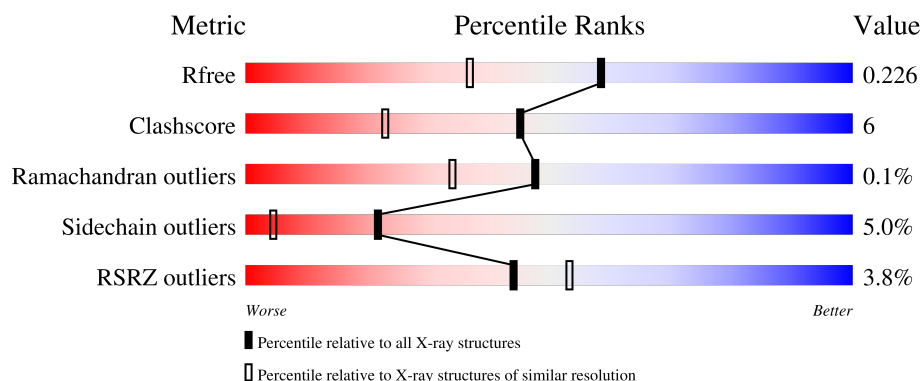
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.73 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}	180053	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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 $\leq 5\%$. 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	233	9% 85% 13% .
1	B	233	3% 88% 11% .
1	C	233	4% 84% 14% ..
1	D	233	87% 12% .
1	E	233	3% 85% 11% ..

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Mol	Chain	Length	Quality of chain
1	F	233	

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	E	301	-	X	-	-
3	TRS	C	302	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12292 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 Purine nucleoside phosphorylase DeoD-type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	2	0
			1810	1154	303	335	18			
1	B	233	Total	C	N	O	S	0	1	0
			1805	1151	302	334	18			
1	C	233	Total	C	N	O	S	0	2	0
			1810	1154	303	335	18			
1	D	233	Total	C	N	O	S	0	2	0
			1811	1155	302	336	18			
1	E	233	Total	C	N	O	S	0	2	0
			1808	1153	302	335	18			
1	F	233	Total	C	N	O	S	0	0	0
			1802	1149	302	334	17			

There are 12 discrepancies between the modelled and reference sequences:

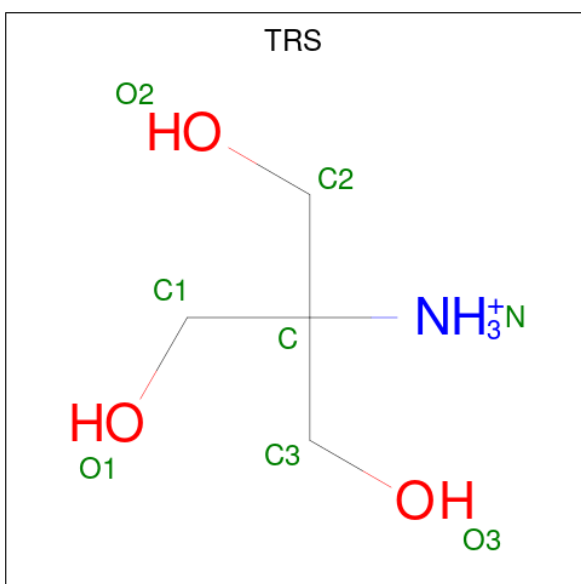
Chain	Residue	Modelled	Actual	Comment	Reference
A	55	ARG	LYS	conflict	UNP I9S9Z7
A	81	GLN	HIS	conflict	UNP I9S9Z7
B	55	ARG	LYS	conflict	UNP I9S9Z7
B	81	GLN	HIS	conflict	UNP I9S9Z7
C	55	ARG	LYS	conflict	UNP I9S9Z7
C	81	GLN	HIS	conflict	UNP I9S9Z7
D	55	ARG	LYS	conflict	UNP I9S9Z7
D	81	GLN	HIS	conflict	UNP I9S9Z7
E	55	ARG	LYS	conflict	UNP I9S9Z7
E	81	GLN	HIS	conflict	UNP I9S9Z7
F	55	ARG	LYS	conflict	UNP I9S9Z7
F	81	GLN	HIS	conflict	UNP I9S9Z7

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



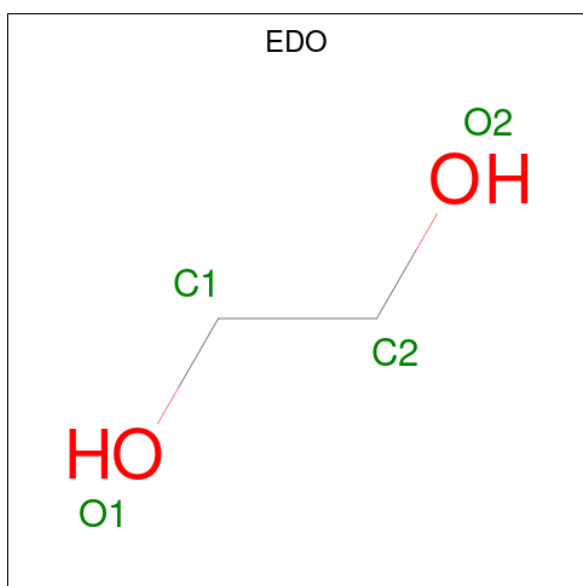
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 8 4 1 3	0	0
3	B	1	Total C N O 8 4 1 3	0	0
3	C	1	Total C N O 8 4 1 3	0	0
3	E	1	Total C N O 8 4 1 3	0	0

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

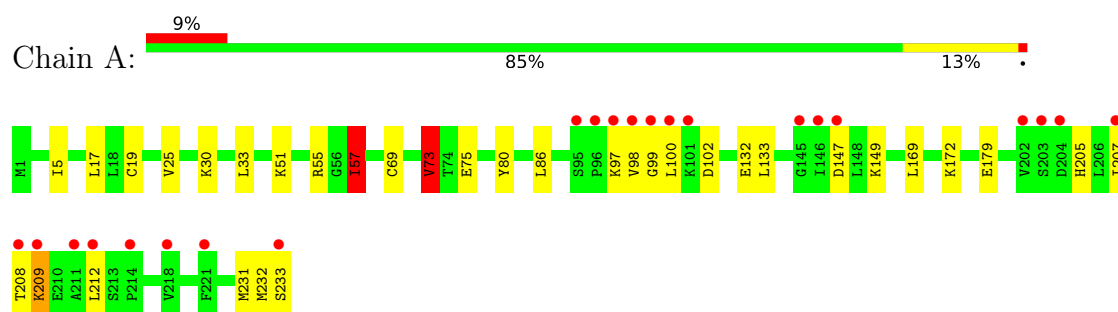
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	230	Total	O	0	0
			230	230		
5	B	225	Total	O	0	0
			225	225		
5	C	245	Total	O	0	0
			245	245		
5	D	234	Total	O	0	0
			234	234		
5	E	209	Total	O	0	0
			209	209		
5	F	211	Total	O	0	0
			211	211		

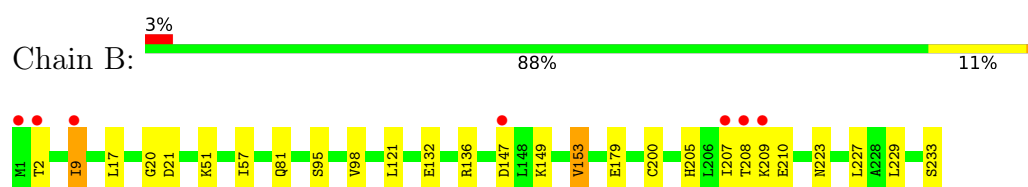
3 Residue-property plots [i](#)

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.

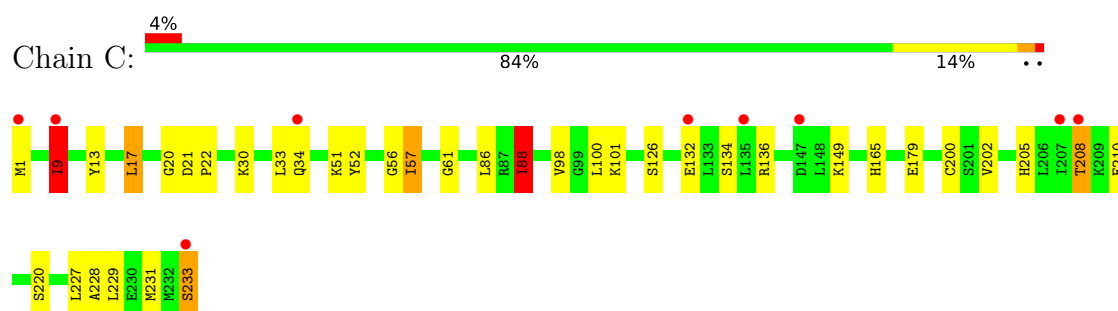
- Molecule 1: Purine nucleoside phosphorylase DeoD-type



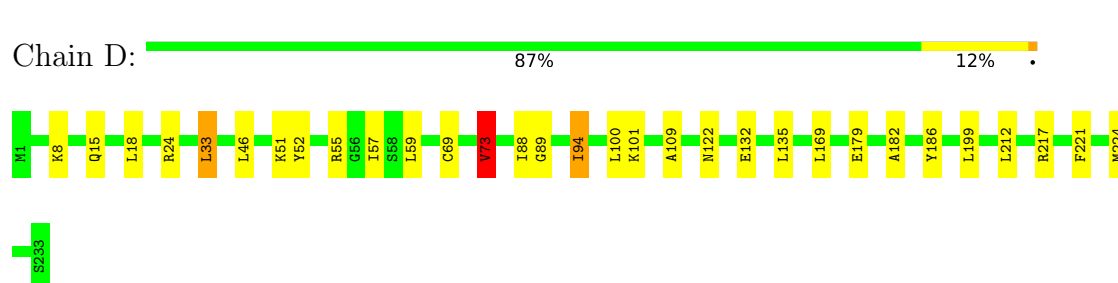
- Molecule 1: Purine nucleoside phosphorylase DeoD-type



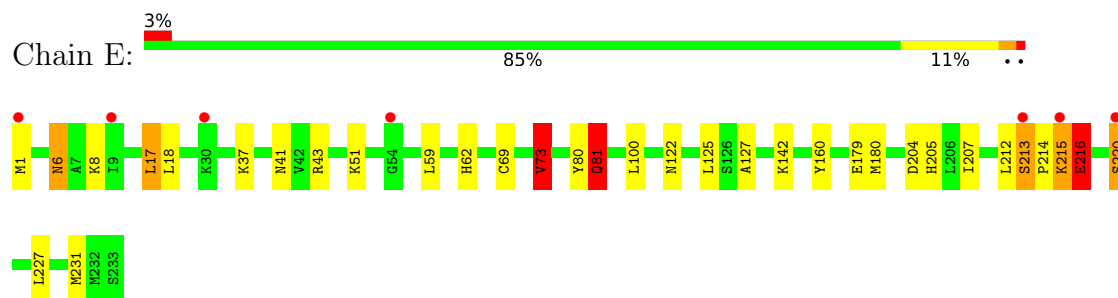
- Molecule 1: Purine nucleoside phosphorylase DeoD-type



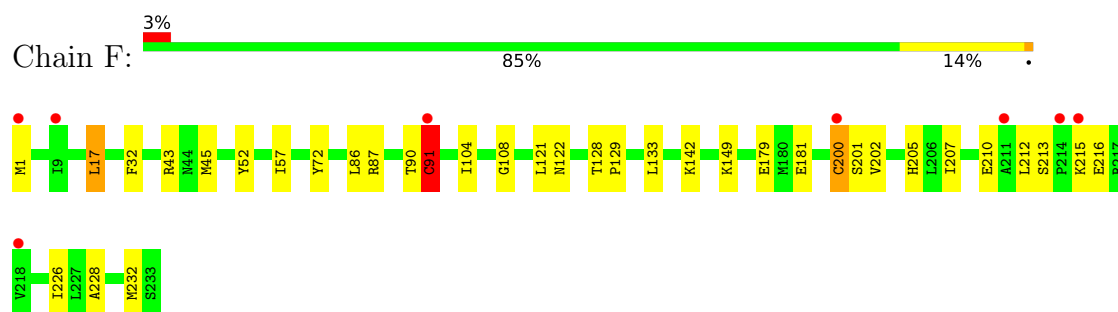
- Molecule 1: Purine nucleoside phosphorylase DeoD-type



- Molecule 1: Purine nucleoside phosphorylase DeoD-type



- Molecule 1: Purine nucleoside phosphorylase DeoD-type



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.52Å 86.31Å 268.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	134.22 – 1.73 134.22 – 1.73	Depositor EDS
% Data completeness (in resolution range)	87.3 (134.22-1.73) 87.3 (134.22-1.73)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 1.73Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.184 , 0.228 0.183 , 0.226	Depositor DCC
R_{free} test set	6228 reflections (4.28%)	wwPDB-VP
Wilson B-factor (Å ²)	13.3	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12292	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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

5.1 Standard geometry

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

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	0.93	0/1847	1.07	5/2486 (0.2%)
1	B	0.90	0/1839	1.04	4/2475 (0.2%)
1	C	0.93	0/1847	1.02	3/2486 (0.1%)
1	D	0.92	0/1848	1.01	1/2487 (0.0%)
1	E	0.89	0/1845	1.10	7/2483 (0.3%)
1	F	0.95	4/1833 (0.2%)	1.29	1/2467 (0.0%)
All	All	0.92	4/11059 (0.0%)	1.09	21/14884 (0.1%)

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	F	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	90	THR	C-N	-10.69	1.19	1.33
1	F	202	VAL	C-O	-7.12	1.16	1.24
1	F	201	SER	C-O	-5.73	1.17	1.24
1	F	200	CYS	C-O	-5.57	1.17	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	91	CYS	O-C-N	-40.95	76.01	123.10
1	A	208	THR	N-CA-C	8.55	125.52	114.75
1	E	213	SER	CA-C-N	8.15	130.02	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	213	SER	C-N-CA	8.15	130.02	119.84
1	E	215	LYS	CA-C-N	8.09	136.25	121.70
1	E	215	LYS	C-N-CA	8.09	136.25	121.70
1	B	153	VAL	CG1-CB-CG2	6.57	125.24	110.80
1	B	153	VAL	N-CA-CB	-6.16	102.12	112.47
1	B	95	SER	CA-C-N	6.14	126.03	119.28
1	B	95	SER	C-N-CA	6.14	126.03	119.28
1	C	9	ILE	N-CA-C	5.80	120.24	111.89
1	E	73	VAL	N-CA-CB	5.65	119.06	110.58
1	A	73	VAL	N-CA-CB	5.41	118.69	110.58
1	A	57	ILE	CB-CA-C	-5.31	101.21	110.71
1	E	215	LYS	N-CA-C	5.27	122.02	110.80
1	C	20	GLY	N-CA-C	-5.13	106.50	113.37
1	C	88	ILE	CB-CA-C	5.11	116.39	111.23
1	D	73	VAL	N-CA-CB	5.10	118.23	110.58
1	E	81	GLN	CB-CA-C	-5.09	102.75	111.26
1	A	208	THR	CA-C-N	5.05	130.80	121.70
1	A	208	THR	C-N-CA	5.05	130.80	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	91	CYS	Mainchain

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	1810	0	1849	28	0
1	B	1805	0	1843	13	0
1	C	1810	0	1849	29	0
1	D	1811	0	1849	23	0
1	E	1808	0	1848	20	0
1	F	1802	0	1838	20	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	0	0
2	E	5	0	0	0	0
3	A	8	0	12	0	0
3	B	8	0	12	0	0
3	C	8	0	12	0	0
3	E	8	0	12	1	0
4	A	4	0	6	0	0
4	B	20	0	30	2	0
4	C	4	0	6	0	0
4	D	4	0	6	0	0
4	E	4	0	6	0	0
4	F	4	0	6	0	0
5	A	230	0	0	13	0
5	B	225	0	0	3	0
5	C	245	0	0	11	0
5	D	234	0	0	12	0
5	E	209	0	0	3	0
5	F	211	0	0	5	0
All	All	12292	0	11184	130	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 (130) 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:94:ILE:HG21	5:D:585:HOH:O	1.36	1.21
1:C:134:SER:HB2	5:C:449:HOH:O	1.42	1.17
1:A:169:LEU:HD12	5:A:516:HOH:O	1.51	1.10
1:F:17:LEU:HD23	1:F:232:MET:SD	1.94	1.07
1:C:202:VAL:HG12	5:C:485:HOH:O	1.53	1.06
1:C:100:LEU:HD12	5:C:485:HOH:O	1.53	1.06
1:C:205:HIS:HB3	1:C:208:THR:HG22	1.43	1.00
1:D:182:ALA:HB1	5:D:560:HOH:O	1.59	1.00
1:D:224:MET:HE3	5:D:530:HOH:O	1.63	0.99
1:D:109:ALA:HB2	5:D:560:HOH:O	1.70	0.91
1:A:75:GLU:HB3	5:A:405:HOH:O	1.71	0.90
1:C:61:GLY:HA3	5:C:405:HOH:O	1.74	0.87
1:A:33:LEU:HD22	1:A:57:ILE:HD11	1.57	0.86
1:C:208:THR:HG21	1:C:210:GLU:OE1	1.80	0.82
1:A:55:ARG:HD3	1:A:233:SER:HA	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ARG:HB3	5:C:402:HOH:O	1.81	0.79
1:C:165:HIS:HD2	5:C:581:HOH:O	1.65	0.78
1:E:125:LEU:HG	5:E:401:HOH:O	1.83	0.77
1:D:24:ARG:HD3	1:D:221:PHE:CZ	2.22	0.74
1:F:17:LEU:CD2	1:F:232:MET:SD	2.75	0.74
1:A:212:LEU:HB2	5:A:412:HOH:O	1.88	0.72
1:D:132[A]:GLU:HG3	5:D:587:HOH:O	1.91	0.71
1:E:127:ALA:HA	5:E:401:HOH:O	1.90	0.70
1:E:216:GLU:O	1:E:220:SER:HB2	1.93	0.68
1:D:186:TYR:CE2	5:D:560:HOH:O	2.46	0.67
1:A:33:LEU:CD2	1:A:57:ILE:HD11	2.24	0.67
1:F:108:GLY:HA2	5:F:424:HOH:O	1.96	0.66
1:D:15:GLN:HE22	1:D:55:ARG:HE	1.43	0.65
1:D:88:ILE:HB	5:D:530:HOH:O	1.97	0.64
4:B:303:EDO:H22	5:B:413:HOH:O	1.98	0.62
1:F:129:PRO:HD3	5:F:424:HOH:O	1.98	0.62
1:E:205:HIS:HD2	1:E:207:ILE:H	1.48	0.62
1:B:205:HIS:HD2	1:B:207:ILE:H	1.48	0.61
4:B:304:EDO:H12	1:E:160:TYR:HB3	1.82	0.61
1:C:132:GLU:HB3	5:C:418:HOH:O	1.99	0.61
1:B:57:ILE:HD13	1:B:229:LEU:HD23	1.83	0.60
1:C:52:TYR:HB2	1:C:57:ILE:HD11	1.82	0.60
1:E:215:LYS:HB3	1:E:216:GLU:HB2	1.84	0.60
1:F:128:THR:HA	5:F:424:HOH:O	2.01	0.59
1:C:100:LEU:HD13	1:C:210:GLU:HG3	1.85	0.59
1:A:30:LYS:HG3	5:A:551:HOH:O	2.02	0.59
1:E:227:LEU:O	1:E:231:MET:HG2	2.03	0.58
1:E:180:MET:HG3	3:E:302:TRS:H11	1.85	0.58
1:D:24:ARG:HD3	1:D:221:PHE:CE1	2.39	0.57
1:A:172:LYS:HB3	5:A:516:HOH:O	2.04	0.57
1:B:132:GLU:O	1:B:136:ARG:HG3	2.05	0.57
1:A:99:GLY:HA2	5:A:428:HOH:O	2.05	0.56
1:E:100:LEU:HD23	1:E:212:LEU:HD23	1.88	0.56
1:F:205:HIS:HD2	1:F:207:ILE:H	1.54	0.56
1:C:101:LYS:HE3	1:C:220:SER:HB3	1.86	0.56
1:B:121:LEU:HD21	1:D:169:LEU:HD23	1.88	0.55
1:F:213:SER:OG	1:F:216:GLU:HG2	2.06	0.55
1:F:52:TYR:HB3	1:F:57:ILE:HD12	1.88	0.55
1:D:89:GLY:HA2	5:D:556:HOH:O	2.07	0.54
1:C:22:PRO:HB3	5:C:405:HOH:O	2.07	0.53
1:F:108:GLY:CA	5:F:424:HOH:O	2.53	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:MET:HB2	5:C:402:HOH:O	2.09	0.52
1:D:186:TYR:CD2	5:D:560:HOH:O	2.63	0.52
1:E:215:LYS:CA	1:E:216:GLU:HB2	2.40	0.52
1:A:5:ILE:HD12	5:A:405:HOH:O	2.09	0.51
1:D:15:GLN:NE2	1:D:55:ARG:HE	2.08	0.51
1:D:52:TYR:HB3	1:D:57:ILE:HD12	1.93	0.51
1:B:233:SER:HB2	5:B:457:HOH:O	2.11	0.51
1:A:86:LEU:HD22	1:A:232:MET:HE3	1.92	0.51
1:C:227:LEU:O	1:C:231:MET:HG2	2.11	0.50
1:F:212:LEU:HB3	1:F:216:GLU:HG3	1.94	0.50
1:A:231:MET:HE2	1:A:232:MET:CE	2.42	0.49
1:C:33:LEU:CD2	1:C:57:ILE:HD11	2.41	0.49
1:C:52:TYR:HB2	1:C:57:ILE:CD1	2.43	0.49
1:C:21:ASP:OD1	1:F:43:ARG:HA	2.13	0.49
1:E:215:LYS:CB	1:E:216:GLU:HB2	2.42	0.48
1:A:80:TYR:HE2	5:A:405:HOH:O	1.96	0.48
1:A:147:ASP:HB2	5:A:569:HOH:O	2.13	0.48
1:D:33:LEU:HD22	1:D:59:LEU:HD11	1.94	0.48
1:C:1:MET:HE2	1:C:9:ILE:CG2	2.44	0.48
1:A:172:LYS:HD3	5:A:516:HOH:O	2.13	0.48
1:A:133:LEU:HD22	1:A:232:MET:HE1	1.96	0.47
1:A:69:CYS:O	1:A:73:VAL:HG13	2.14	0.47
1:A:132:GLU:HG2	5:A:451:HOH:O	2.14	0.47
1:D:217:ARG:HD3	5:D:521:HOH:O	2.14	0.47
1:A:98:VAL:HG12	1:A:149:LYS:HG3	1.97	0.47
1:A:99:GLY:O	1:A:102:ASP:HB2	2.15	0.47
1:C:98:VAL:HG12	1:C:149:LYS:HG3	1.97	0.47
1:F:17:LEU:HD22	1:F:86:LEU:HB3	1.96	0.47
1:B:98:VAL:HG12	1:B:149:LYS:HG3	1.98	0.46
1:C:57:ILE:HD12	1:C:229:LEU:CD2	2.45	0.46
1:F:17:LEU:HD21	1:F:228:ALA:HB1	1.98	0.46
1:F:87:ARG:NH2	1:F:181:GLU:OE1	2.48	0.46
1:C:17:LEU:HD12	1:C:86:LEU:HB3	1.97	0.46
1:B:205:HIS:CD2	1:B:208:THR:H	2.35	0.45
1:A:97:LYS:HE2	5:A:401:HOH:O	2.16	0.45
1:E:6:ASN:H	1:E:6:ASN:HD22	1.65	0.45
1:F:32:PHE:HE1	1:F:226:ILE:HD11	1.82	0.45
1:D:69:CYS:O	1:D:73:VAL:HG13	2.17	0.44
1:C:57:ILE:HD12	1:C:229:LEU:HD22	1.98	0.44
1:E:17:LEU:HB2	1:E:59:LEU:HD23	1.98	0.44
1:A:205:HIS:CE1	1:A:207:ILE:HG13	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:HIS:HE1	1:A:207:ILE:HG13	1.81	0.44
1:B:147:ASP:HB3	5:B:401:HOH:O	2.18	0.44
1:C:88:ILE:HG21	1:C:228:ALA:HB2	2.00	0.44
1:D:212:LEU:HB2	1:D:217:ARG:HG3	1.99	0.43
1:A:19:CYS:HB2	1:A:25:VAL:HG23	1.99	0.43
1:E:6:ASN:HD21	1:E:41:ASN:H	1.66	0.43
1:F:45:MET:HG2	1:F:72:TYR:CZ	2.53	0.43
1:F:91:CYS:SG	1:F:200:CYS:HB3	2.58	0.43
1:C:13:TYR:CE1	1:C:56:GLY:HA3	2.54	0.43
1:D:88:ILE:HG22	1:D:199:LEU:HB2	2.01	0.43
1:E:80:TYR:O	1:E:81:GLN:HB2	2.19	0.43
1:E:18:LEU:HB3	1:E:62:HIS:HD2	1.84	0.43
1:E:69:CYS:O	1:E:73:VAL:HG13	2.19	0.43
1:F:1:MET:N	5:F:403:HOH:O	2.51	0.42
1:B:223:ASN:HD22	1:B:223:ASN:HA	1.66	0.42
1:B:21:ASP:OD1	1:E:43:ARG:HA	2.20	0.42
1:B:9:ILE:H	1:B:9:ILE:HG13	1.75	0.42
1:B:20:GLY:HA3	2:B:301:PO4:O4	2.20	0.42
1:A:169:LEU:HD23	1:F:121:LEU:HD21	2.01	0.42
1:A:205:HIS:O	1:A:209:LYS:HA	2.20	0.41
1:B:205:HIS:CD2	1:B:207:ILE:H	2.34	0.41
1:E:213:SER:O	1:E:215:LYS:N	2.54	0.41
1:C:233:SER:HB3	5:C:438:HOH:O	2.20	0.41
1:D:221:PHE:CZ	5:D:530:HOH:O	2.57	0.41
1:E:213:SER:O	1:E:216:GLU:CB	2.68	0.41
1:A:55:ARG:HD3	1:A:233:SER:CA	2.42	0.41
1:D:18:LEU:HD13	5:D:564:HOH:O	2.21	0.41
1:C:126:SER:HB2	5:E:444:HOH:O	2.21	0.41
1:C:208:THR:HG23	1:C:210:GLU:H	1.85	0.41
1:C:136:ARG:HD3	5:C:418:HOH:O	2.21	0.40
1:D:100:LEU:O	1:D:101:LYS:HB2	2.22	0.40
1:F:104:ILE:HA	1:F:149:LYS:O	2.21	0.40
1:A:205:HIS:CD2	5:A:428:HOH:O	2.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	233/233 (100%)	224 (96%)	9 (4%)	0	100	100
1	B	232/233 (100%)	225 (97%)	7 (3%)	0	100	100
1	C	233/233 (100%)	225 (97%)	8 (3%)	0	100	100
1	D	233/233 (100%)	225 (97%)	8 (3%)	0	100	100
1	E	233/233 (100%)	224 (96%)	7 (3%)	2 (1%)	14	3
1	F	231/233 (99%)	226 (98%)	5 (2%)	0	100	100
All	All	1395/1398 (100%)	1349 (97%)	44 (3%)	2 (0%)	48	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	214	PRO
1	E	216	GLU

5.3.2 Protein sidechains

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	198/196 (101%)	191 (96%)	7 (4%)	32	9
1	B	197/196 (100%)	185 (94%)	12 (6%)	17	2
1	C	198/196 (101%)	186 (94%)	12 (6%)	17	2
1	D	198/196 (101%)	189 (96%)	9 (4%)	24	5
1	E	198/196 (101%)	184 (93%)	14 (7%)	13	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	196/196 (100%)	189 (96%)	7 (4%)	31 9
All	All	1185/1176 (101%)	1124 (95%)	61 (5%)	22 4

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	51	LYS
1	A	57	ILE
1	A	73	VAL
1	A	100	LEU
1	A	179	GLU
1	A	209	LYS
1	B	2	THR
1	B	9	ILE
1	B	17	LEU
1	B	51	LYS
1	B	81	GLN
1	B	153	VAL
1	B	179	GLU
1	B	200[A]	CYS
1	B	200[B]	CYS
1	B	209	LYS
1	B	210	GLU
1	B	227	LEU
1	C	9	ILE
1	C	17	LEU
1	C	30	LYS
1	C	34	GLN
1	C	51	LYS
1	C	57	ILE
1	C	88	ILE
1	C	179	GLU
1	C	200[A]	CYS
1	C	200[B]	CYS
1	C	208	THR
1	C	233	SER
1	D	8	LYS
1	D	33	LEU
1	D	46	LEU
1	D	51	LYS
1	D	73	VAL

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Mol	Chain	Res	Type
1	D	94	ILE
1	D	122	ASN
1	D	135	LEU
1	D	179	GLU
1	E	1	MET
1	E	6	ASN
1	E	8	LYS
1	E	17	LEU
1	E	37	LYS
1	E	51	LYS
1	E	73	VAL
1	E	81	GLN
1	E	122	ASN
1	E	142	LYS
1	E	179	GLU
1	E	204	ASP
1	E	216	GLU
1	E	220	SER
1	F	17	LEU
1	F	122	ASN
1	F	133	LEU
1	F	142	LYS
1	F	179	GLU
1	F	210	GLU
1	F	215	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	HIS
1	B	34	GLN
1	B	205	HIS
1	B	223	ASN
1	C	34	GLN
1	C	165	HIS
1	D	15	GLN
1	E	6	ASN
1	E	205	HIS
1	F	15	GLN
1	F	205	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

18 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	B	301	-	4,4,4	0.80	0	6,6,6	0.51	0
3	TRS	E	302	-	7,7,7	0.63	0	9,9,9	0.86	0
4	EDO	C	303	-	3,3,3	0.31	0	2,2,2	0.49	0
4	EDO	B	306	-	3,3,3	0.39	0	2,2,2	0.32	0
4	EDO	B	307	-	3,3,3	0.54	0	2,2,2	0.17	0
2	PO4	A	301	-	4,4,4	0.86	0	6,6,6	1.50	1 (16%)
2	PO4	E	301	-	4,4,4	1.79	2 (50%)	6,6,6	1.65	2 (33%)
3	TRS	A	302	-	7,7,7	0.63	0	9,9,9	1.24	2 (22%)
3	TRS	B	302	-	7,7,7	0.61	0	9,9,9	0.93	0
4	EDO	B	303	-	3,3,3	0.63	0	2,2,2	0.51	0
4	EDO	B	304	-	3,3,3	0.56	0	2,2,2	0.32	0
4	EDO	B	305	-	3,3,3	0.37	0	2,2,2	0.67	0
4	EDO	A	303	-	3,3,3	0.52	0	2,2,2	0.34	0
3	TRS	C	302	-	7,7,7	0.86	0	9,9,9	4.88	8 (88%)
4	EDO	E	303	-	3,3,3	0.54	0	2,2,2	0.60	0
2	PO4	C	301	-	4,4,4	0.82	0	6,6,6	0.72	0
4	EDO	F	301	-	3,3,3	0.54	0	2,2,2	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	D	301	-	3,3,3	0.57	0	2,2,2	0.54	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
3	TRS	E	302	-	-	0/9/9/9	-
4	EDO	E	303	-	-	0/1/1/1	-
4	EDO	B	306	-	-	0/1/1/1	-
4	EDO	B	307	-	-	1/1/1/1	-
3	TRS	A	302	-	-	2/9/9/9	-
4	EDO	B	303	-	-	1/1/1/1	-
3	TRS	B	302	-	-	2/9/9/9	-
4	EDO	B	304	-	-	1/1/1/1	-
4	EDO	B	305	-	-	1/1/1/1	-
4	EDO	A	303	-	-	0/1/1/1	-
3	TRS	C	302	-	-	6/9/9/9	-
4	EDO	F	301	-	-	0/1/1/1	-
4	EDO	C	303	-	-	0/1/1/1	-
4	EDO	D	301	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	PO4	P-O3	-2.44	1.47	1.54
2	E	301	PO4	P-O1	2.06	1.55	1.50

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	302	TRS	C3-C-N	-7.60	88.80	108.17
3	C	302	TRS	C1-C-N	-7.04	90.22	108.17
3	C	302	TRS	C2-C-N	-6.03	92.80	108.17
3	C	302	TRS	C2-C-C1	5.90	126.38	110.66
3	C	302	TRS	O1-C1-C	3.38	120.30	110.88
2	A	301	PO4	O3-P-O2	3.21	117.92	107.91
3	C	302	TRS	O2-C2-C	2.87	118.87	110.88
2	E	301	PO4	O2-P-O1	-2.84	100.91	110.95
3	C	302	TRS	C3-C-C2	2.83	118.20	110.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	301	PO4	O4-P-O2	2.40	115.39	107.91
3	C	302	TRS	O3-C3-C	2.29	117.27	110.88
3	A	302	TRS	C2-C-N	2.19	113.75	108.17
3	A	302	TRS	C2-C-C1	-2.07	105.15	110.66

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	302	TRS	C1-C-C2-O2
3	C	302	TRS	N-C-C2-O2
3	C	302	TRS	C2-C-C3-O3
3	C	302	TRS	C2-C-C1-O1
4	B	303	EDO	O1-C1-C2-O2
4	B	307	EDO	O1-C1-C2-O2
3	C	302	TRS	C3-C-C1-O1
4	B	305	EDO	O1-C1-C2-O2
3	B	302	TRS	C2-C-C3-O3
3	C	302	TRS	N-C-C3-O3
4	B	304	EDO	O1-C1-C2-O2
3	A	302	TRS	C3-C-C1-O1
3	A	302	TRS	C1-C-C3-O3
3	B	302	TRS	C1-C-C3-O3

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	PO4	1	0
3	E	302	TRS	1	0
4	B	303	EDO	1	0
4	B	304	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	90:THR	C	91:CYS	N	1.19

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	233/233 (100%)	0.12	22 (9%) 14 18	6, 12, 37, 55	2 (0%)
1	B	233/233 (100%)	-0.15	7 (3%) 52 61	5, 12, 27, 48	1 (0%)
1	C	233/233 (100%)	0.08	9 (3%) 43 52	6, 15, 28, 38	2 (0%)
1	D	233/233 (100%)	-0.21	0 100 100	5, 11, 29, 42	2 (0%)
1	E	233/233 (100%)	0.02	7 (3%) 52 61	6, 14, 31, 57	2 (0%)
1	F	233/233 (100%)	0.04	8 (3%) 48 56	7, 15, 33, 48	0
All	All	1398/1398 (100%)	-0.02	53 (3%) 44 53	5, 13, 31, 57	9 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	213	SER	5.6
1	A	208	THR	5.3
1	A	100	LEU	5.2
1	B	207	ILE	5.1
1	A	211	ALA	4.6
1	F	211	ALA	4.5
1	B	9	ILE	4.1
1	A	98	VAL	3.8
1	A	204	ASP	3.6
1	F	214	PRO	3.5
1	A	207	ILE	3.5
1	C	147	ASP	3.4
1	A	99	GLY	3.4
1	E	215	LYS	3.3
1	B	1	MET	3.1
1	F	91	CYS	3.0
1	A	147	ASP	2.8
1	C	233	SER	2.8
1	B	2	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	96	PRO	2.7
1	A	146	ILE	2.7
1	E	1	MET	2.7
1	C	207	ILE	2.6
1	E	9	ILE	2.5
1	A	145	GLY	2.4
1	A	203	SER	2.4
1	A	214	PRO	2.4
1	C	135	LEU	2.4
1	F	9	ILE	2.4
1	F	218	VAL	2.4
1	A	95	SER	2.3
1	C	9	ILE	2.3
1	A	209	LYS	2.3
1	B	147	ASP	2.3
1	A	101	LYS	2.2
1	F	215	LYS	2.2
1	E	30	LYS	2.2
1	A	221	PHE	2.2
1	A	202	VAL	2.2
1	C	208	THR	2.2
1	A	218	VAL	2.1
1	F	200	CYS	2.1
1	C	1	MET	2.1
1	E	54	GLY	2.1
1	A	212	LEU	2.1
1	C	34	GLN	2.1
1	E	220	SER	2.1
1	B	208	THR	2.1
1	F	1	MET	2.1
1	B	209	LYS	2.1
1	C	132	GLU	2.0
1	A	97	LYS	2.0
1	A	233	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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
4	EDO	B	303	4/4	0.83	0.25	75,77,82,89	0
3	TRS	E	302	8/8	0.84	0.14	20,24,25,29	0
4	EDO	B	306	4/4	0.87	0.14	38,39,39,43	0
4	EDO	B	307	4/4	0.87	0.15	29,29,29,35	0
4	EDO	C	303	4/4	0.88	0.18	39,44,46,48	0
4	EDO	B	304	4/4	0.92	0.11	21,23,26,27	0
2	PO4	A	301	5/5	0.93	0.13	18,19,20,21	0
3	TRS	C	302	8/8	0.94	0.07	12,13,14,15	0
3	TRS	A	302	8/8	0.94	0.08	16,21,22,24	0
4	EDO	B	305	4/4	0.94	0.11	24,30,31,34	0
4	EDO	F	301	4/4	0.94	0.07	18,19,20,21	0
4	EDO	A	303	4/4	0.96	0.07	18,19,20,22	0
4	EDO	E	303	4/4	0.96	0.06	16,16,17,17	0
3	TRS	B	302	8/8	0.96	0.06	13,14,14,15	0
4	EDO	D	301	4/4	0.97	0.05	16,17,17,18	0
2	PO4	C	301	5/5	0.98	0.04	10,11,11,12	0
2	PO4	E	301	5/5	0.98	0.04	14,14,15,15	0
2	PO4	B	301	5/5	0.99	0.03	9,9,10,10	0

6.5 Other polymers [i](#)

There are no such residues in this entry.