



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:31 PM UTC

PDB ID : 7R69 / pdb_00007r69
Title : Crystal structure of mutant R43D/C273S of L-Asparaginase I from *Yersinia pestis*
Authors : Strzelczyk, P.; Wlodawer, A.; Lubkowski, J.
Deposited on : 2021-06-22
Resolution : 1.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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

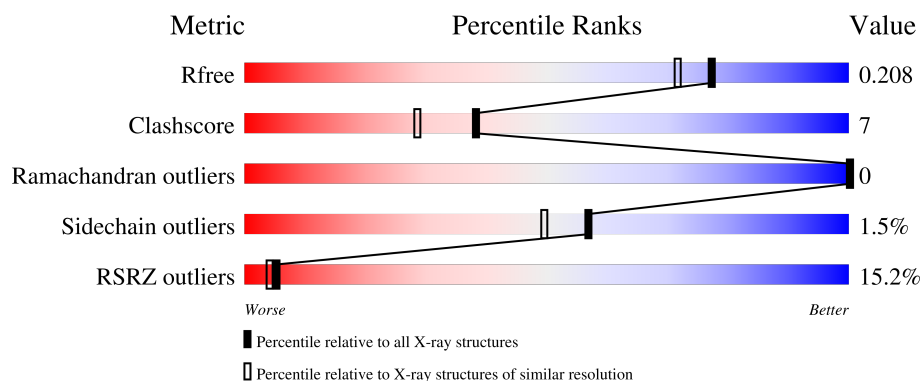
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	338	8% 80% 14% • 6%
1	B	338	10% 81% 10% • 8%
1	C	338	12% 76% 15% • 9%
1	D	338	26% 72% 17% • 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10679 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 I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	319	Total	C	N	O	S	0	8	0
			2468	1565	420	474	9			
1	B	312	Total	C	N	O	S	0	4	0
			2411	1530	412	460	9			
1	C	308	Total	C	N	O	S	0	5	0
			2390	1519	408	454	9			
1	D	303	Total	C	N	O	S	0	2	0
			2337	1485	398	445	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP A0A3N4B0Q2
A	43	ASP	ARG	engineered mutation	UNP A0A3N4B0Q2
A	273	SER	CYS	engineered mutation	UNP A0A3N4B0Q2
B	1	GLY	-	expression tag	UNP A0A3N4B0Q2
B	43	ASP	ARG	engineered mutation	UNP A0A3N4B0Q2
B	273	SER	CYS	engineered mutation	UNP A0A3N4B0Q2
C	1	GLY	-	expression tag	UNP A0A3N4B0Q2
C	43	ASP	ARG	engineered mutation	UNP A0A3N4B0Q2
C	273	SER	CYS	engineered mutation	UNP A0A3N4B0Q2
D	1	GLY	-	expression tag	UNP A0A3N4B0Q2
D	43	ASP	ARG	engineered mutation	UNP A0A3N4B0Q2
D	273	SER	CYS	engineered mutation	UNP A0A3N4B0Q2

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



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	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		
2	D	1	Total	C	O	0	0
			4	2	2		

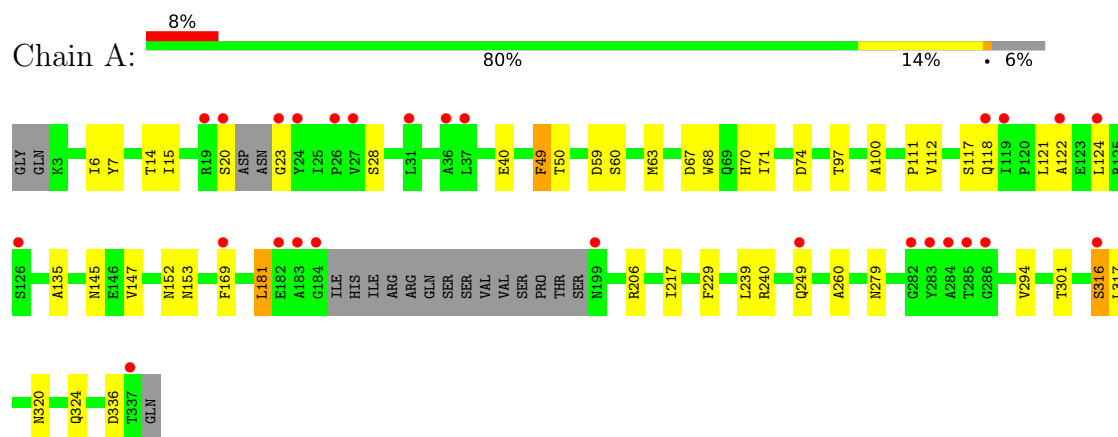
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	344	Total 344	O 344	0	0
3	B	307	Total 307	O 307	0	0
3	C	226	Total 226	O 226	0	0
3	D	144	Total 144	O 144	0	0

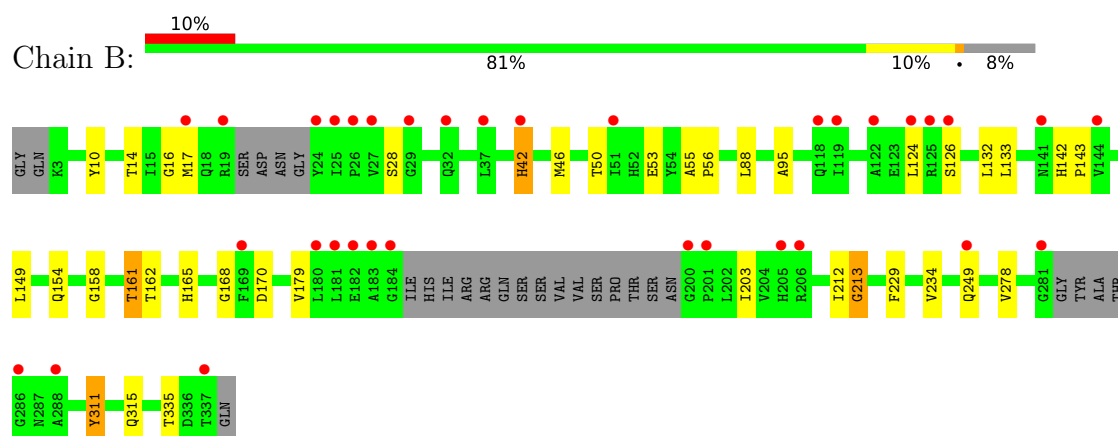
3 Residue-property plots [i](#)

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.

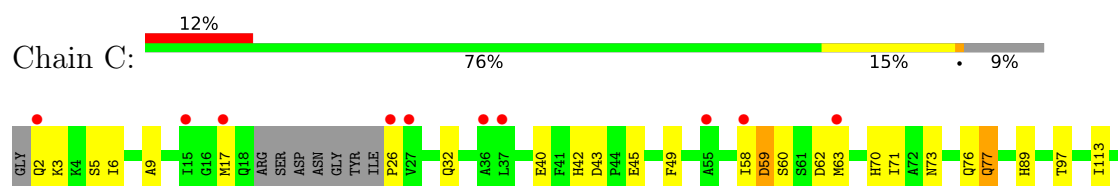
• Molecule 1: L-asparaginase I

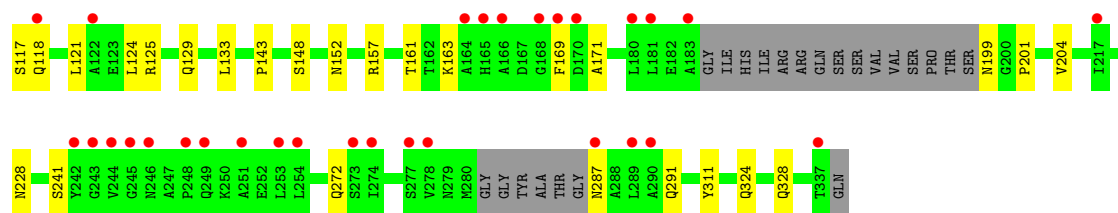


• Molecule 1: L-asparaginase I

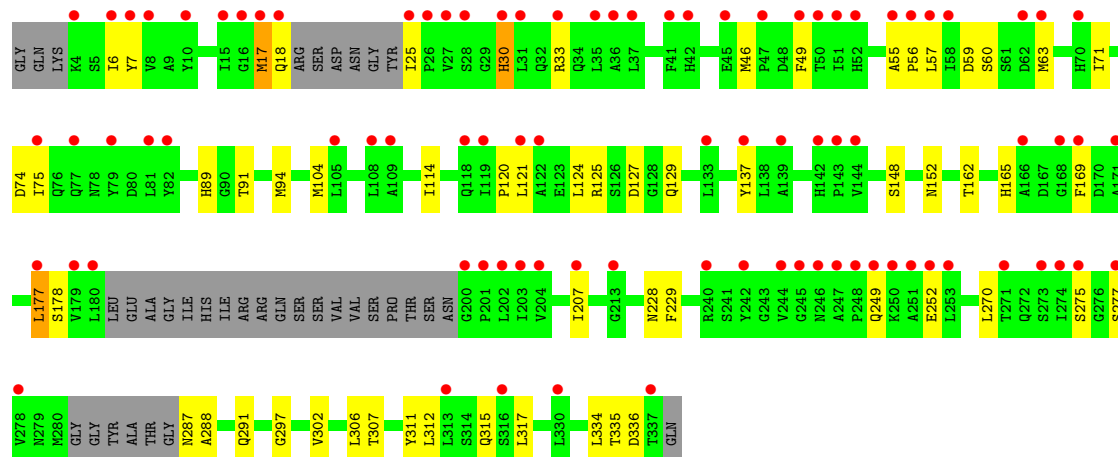
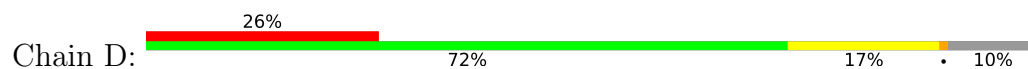


• Molecule 1: L-asparaginase I





● Molecule 1: L-asparaginase I



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.98Å 162.98Å 73.26Å 90.00° 110.39° 90.00°	Depositor
Resolution (Å)	41.12 – 1.80 41.12 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.1 (41.12-1.80) 96.2 (41.12-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.167 , 0.196 0.180 , 0.208	Depositor DCC
R_{free} test set	1882 reflections (1.38%)	wwPDB-VP
Wilson B-factor (Å ²)	18.1	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10679	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% 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

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	1.36	13/2545 (0.5%)	1.40	17/3463 (0.5%)
1	B	1.31	5/2470 (0.2%)	1.41	8/3359 (0.2%)
1	C	1.26	4/2457 (0.2%)	1.43	10/3341 (0.3%)
1	D	1.24	5/2391 (0.2%)	1.43	4/3254 (0.1%)
All	All	1.29	27/9863 (0.3%)	1.42	39/13417 (0.3%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	71	ILE	C-O	7.28	1.32	1.24
1	A	147	VAL	C-O	6.84	1.30	1.23
1	B	234	VAL	C-O	6.73	1.30	1.24
1	C	5	SER	C-O	6.63	1.31	1.24
1	A	317	LEU	C-O	6.47	1.31	1.23
1	A	135	ALA	C-O	6.42	1.31	1.24
1	A	111	PRO	C-O	-6.37	1.17	1.23
1	A	71	ILE	C-O	6.10	1.30	1.24
1	D	275	SER	C-O	6.00	1.31	1.23
1	D	277	SER	C-O	5.99	1.31	1.23
1	A	294	VAL	C-O	5.82	1.31	1.24
1	A	70	HIS	CE1-NE2	5.79	1.38	1.32
1	B	311	TYR	C-O	5.77	1.30	1.24
1	A	67	ASP	C-O	5.68	1.30	1.24
1	D	307	THR	C-O	5.63	1.30	1.24
1	B	126	SER	C-O	5.61	1.30	1.23
1	A	260	ALA	C-O	5.58	1.30	1.24
1	C	143	PRO	C-O	-5.53	1.17	1.23
1	C	9	ALA	CA-CB	-5.39	1.46	1.52
1	B	168	GLY	C-O	5.35	1.30	1.23
1	A	7	TYR	C-O	5.32	1.30	1.24
1	A	279	ASN	C-O	5.22	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	62	ASP	C-O	-5.19	1.17	1.24
1	B	42	HIS	CE1-NE2	5.15	1.37	1.32
1	A	59	ASP	C-O	5.14	1.30	1.23
1	A	316	SER	C-O	5.08	1.30	1.23
1	D	75	ILE	C-O	-5.07	1.18	1.24

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	ASP	CA-C-N	6.71	133.78	121.70
1	A	336	ASP	C-N-CA	6.71	133.78	121.70
1	C	118	GLN	CB-CG-CD	6.56	123.76	112.60
1	C	89	HIS	CA-CB-CG	6.36	120.16	113.80
1	A	40	GLU	CB-CG-CD	6.16	123.08	112.60
1	C	77	GLN	CB-CG-CD	6.13	123.02	112.60
1	B	203	ILE	CA-C-O	-6.07	113.57	120.67
1	A	320	ASN	CA-CB-CG	-6.01	106.58	112.60
1	C	59	ASP	N-CA-CB	5.90	118.80	109.71
1	A	153	ASN	CA-CB-CG	-5.82	106.78	112.60
1	C	42	HIS	CA-CB-CG	-5.68	108.12	113.80
1	C	62	ASP	CA-C-O	-5.59	113.35	119.95
1	A	74	ASP	CA-CB-CG	5.58	118.18	112.60
1	C	143	PRO	CA-C-O	-5.55	115.29	121.23
1	A	320	ASN	CA-C-O	-5.54	114.68	120.55
1	B	335	THR	CA-C-N	-5.53	114.98	122.95
1	B	335	THR	C-N-CA	-5.53	114.98	122.95
1	D	127	ASP	N-CA-C	-5.52	106.04	112.89
1	A	112	VAL	CA-C-O	-5.37	114.85	120.27
1	B	162	THR	CA-CB-OG1	-5.36	101.57	109.60
1	A	49	PHE	CA-C-O	-5.33	115.58	121.33
1	C	71	ILE	CA-C-O	-5.32	115.54	121.17
1	A	50	THR	CA-C-O	-5.31	114.43	120.32
1	D	302	VAL	N-CA-C	-5.25	105.27	110.62
1	D	120	PRO	CA-C-N	5.23	127.55	120.38
1	D	120	PRO	C-N-CA	5.23	127.55	120.38
1	A	100	ALA	CA-C-O	-5.20	115.36	120.82
1	A	316	SER	CA-C-O	-5.17	115.79	121.58
1	A	336	ASP	O-C-N	5.16	129.72	123.01
1	B	212	ILE	CA-C-N	-5.14	117.31	122.20
1	B	212	ILE	C-N-CA	-5.14	117.31	122.20
1	B	213	GLY	CA-C-O	-5.13	116.45	120.91
1	B	229	PHE	CA-C-O	-5.12	114.31	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	229	PHE	CB-CA-C	-5.12	101.17	110.63
1	A	117	SER	O-C-N	5.11	128.89	123.42
1	C	117	SER	O-C-N	5.07	128.59	123.26
1	C	77	GLN	CG-CD-NE2	-5.06	108.80	116.40
1	A	117	SER	CA-C-O	-5.01	115.87	121.23
1	A	68	TRP	N-CA-C	-5.01	105.71	111.07

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	2468	0	2443	19	0
1	B	2411	0	2392	26	0
1	C	2390	0	2375	34	0
1	D	2337	0	2321	52	0
2	A	16	0	24	3	0
2	B	16	0	24	5	0
2	C	12	0	18	3	0
2	D	8	0	12	1	0
3	A	344	0	0	10	0
3	B	307	0	0	7	0
3	C	226	0	0	12	0
3	D	144	0	0	4	0
All	All	10679	0	9609	134	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 7.

All (134) 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:104:MET:CE	1:D:207:ILE:HG21	1.80	1.12
1:D:104:MET:CE	1:D:207:ILE:CG2	2.35	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:MET:HE1	1:D:207:ILE:HG21	1.44	0.96
2:A:404:EDO:H22	3:A:570:HOH:O	1.74	0.86
2:A:404:EDO:C2	3:A:570:HOH:O	2.25	0.83
1:D:104:MET:HE3	1:D:207:ILE:CD1	2.12	0.79
1:B:165[A]:HIS:CE1	1:B:170:ASP:OD2	2.36	0.78
1:C:43:ASP:OD2	1:C:45:GLU:HG3	1.84	0.78
1:D:336:ASP:HB3	3:D:534:HOH:O	1.84	0.76
1:D:104:MET:HE2	1:D:207:ILE:CG2	2.14	0.76
1:A:217:ILE:HD11	1:A:239:LEU:HD22	1.69	0.73
1:B:249:GLN:NE2	3:B:503:HOH:O	2.22	0.73
1:B:42:HIS:HE1	3:B:679:HOH:O	1.70	0.72
1:B:42:HIS:CE1	3:B:679:HOH:O	2.43	0.71
2:B:404:EDO:H21	3:B:681:HOH:O	1.91	0.71
2:D:401:EDO:H22	3:D:544:HOH:O	1.92	0.70
1:B:124:LEU:HD21	1:D:46:MET:HE3	1.72	0.70
1:B:315:GLN:HE22	2:B:403:EDO:H11	1.58	0.68
1:B:165[A]:HIS:HE1	1:B:170:ASP:OD2	1.77	0.68
1:D:104:MET:HE3	1:D:207:ILE:HD13	1.75	0.67
1:C:60:SER:HA	1:C:63:MET:HG2	1.76	0.67
1:D:104:MET:CE	1:D:207:ILE:CB	2.73	0.66
1:C:17:MET:HG2	1:C:26:PRO:N	2.12	0.65
1:D:104:MET:HE2	1:D:207:ILE:HB	1.79	0.65
1:D:46:MET:HA	1:D:46:MET:HE2	1.78	0.65
1:D:104:MET:HE3	1:D:207:ILE:HG21	1.77	0.62
1:D:104:MET:HE1	1:D:207:ILE:CG2	2.18	0.62
1:D:104:MET:CE	1:D:207:ILE:HB	2.29	0.62
1:D:177:LEU:HD13	1:D:178:SER:N	2.14	0.61
2:C:402:EDO:H11	3:C:628:HOH:O	1.99	0.61
1:C:40:GLU:OE2	1:C:129:GLN:NE2	2.31	0.61
1:B:46:MET:HE2	1:B:133:LEU:HD12	1.84	0.60
1:C:59:ASP:CB	3:C:508:HOH:O	2.49	0.60
1:D:311:TYR:O	1:D:315:GLN:HG2	2.02	0.60
1:C:241:SER:O	1:C:272:GLN:HG3	2.03	0.59
1:B:311:TYR:CE2	2:B:403:EDO:H22	2.38	0.58
1:D:104:MET:HE2	1:D:207:ILE:CB	2.33	0.58
1:C:201:PRO:HD2	3:C:566:HOH:O	2.02	0.58
1:B:95:ALA:CB	1:B:161[A]:THR:HG23	2.35	0.57
1:C:70[B]:HIS:HD2	3:C:601:HOH:O	1.86	0.57
1:B:278:VAL:O	2:B:401:EDO:H22	2.05	0.56
1:C:77:GLN:HG2	3:C:671:HOH:O	2.05	0.56
1:C:324:GLN:OE1	1:C:328:GLN:NE2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:30:HIS:HD2	1:D:33:ARG:NH2	2.04	0.55
1:B:311:TYR:HE2	2:B:403:EDO:H22	1.71	0.54
1:A:20:SER:N	1:A:23:GLY:O	2.40	0.54
1:D:46:MET:HE1	1:D:137:TYR:HB2	1.90	0.54
1:C:59:ASP:HB2	3:C:508:HOH:O	2.08	0.54
3:C:516:HOH:O	1:D:229:PHE:HE1	1.91	0.54
1:B:154:GLN:NE2	3:B:507:HOH:O	2.41	0.54
1:C:70[B]:HIS:CD2	3:C:601:HOH:O	2.60	0.53
1:D:104:MET:HE3	1:D:207:ILE:CB	2.40	0.52
1:C:311:TYR:OH	2:C:401:EDO:H22	2.10	0.52
1:C:73:ASN:OD1	2:C:403:EDO:H11	2.10	0.52
1:D:121:LEU:HD12	1:D:129:GLN:HA	1.92	0.52
1:D:177:LEU:HD12	1:D:178:SER:O	2.10	0.52
1:A:152:ASN:HB2	1:A:169:PHE:O	2.10	0.51
1:C:201:PRO:CD	3:C:566:HOH:O	2.59	0.51
1:D:177:LEU:CD1	1:D:178:SER:O	2.58	0.51
1:D:249:GLN:HE22	1:D:288:ALA:CB	2.23	0.51
1:C:63:MET:HE2	1:C:97:THR:OG1	2.10	0.51
1:C:287:ASN:O	1:C:291:GLN:HG2	2.10	0.51
1:D:30:HIS:CD2	1:D:33:ARG:NH2	2.79	0.50
1:D:60:SER:O	1:D:63:MET:HB2	2.12	0.49
1:C:70[A]:HIS:HE1	3:C:695:HOH:O	1.94	0.49
1:C:113:ILE:HG12	1:C:148[B]:SER:OG	2.11	0.49
1:B:142:HIS:N	1:B:143:PRO:CD	2.75	0.48
1:D:124:LEU:HG	1:D:125:ARG:HG3	1.95	0.48
1:C:58:ILE:HG21	1:C:63:MET:SD	2.53	0.48
1:D:91:THR:HA	1:D:94:MET:HE3	1.94	0.48
1:A:324:GLN:HG2	3:A:566:HOH:O	2.13	0.48
1:B:149:LEU:HD13	1:B:161[A]:THR:HG21	1.96	0.48
1:D:46:MET:CE	1:D:137:TYR:HD1	2.27	0.47
1:A:60:SER:HA	1:A:63:MET:HG2	1.95	0.47
1:A:145:ASN:ND2	3:A:508:HOH:O	2.47	0.47
1:C:70[A]:HIS:ND1	3:C:504:HOH:O	2.46	0.47
1:D:104:MET:HE3	1:D:207:ILE:HD12	1.95	0.47
1:C:163:LYS:NZ	1:C:171:ALA:HB1	2.29	0.47
1:D:249:GLN:HE22	1:D:288:ALA:HB2	1.79	0.47
1:A:124:LEU:O	3:A:501:HOH:O	2.20	0.47
1:C:157:ARG:O	1:C:161:THR:HG23	2.15	0.47
1:B:50:THR:OG1	3:B:502:HOH:O	2.20	0.46
1:C:287:ASN:O	1:C:291:GLN:CG	2.63	0.46
1:D:17:MET:HE3	1:D:25:ILE:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ALA:CB	3:A:541:HOH:O	2.63	0.46
1:A:181:LEU:C	1:A:181:LEU:HD12	2.40	0.46
1:C:152:ASN:HB2	1:C:169:PHE:O	2.16	0.46
1:D:287:ASN:C	1:D:291:GLN:HE21	2.24	0.46
1:A:240:ARG:NH2	3:A:507:HOH:O	2.47	0.46
1:B:158:GLY:O	1:B:161[A]:THR:HG22	2.16	0.45
1:D:306:LEU:C	1:D:306:LEU:HD13	2.41	0.45
1:D:121:LEU:HD12	1:D:129:GLN:CA	2.46	0.45
1:D:104:MET:HE2	1:D:207:ILE:HG22	1.95	0.45
1:D:114:ILE:HG22	1:D:148:SER:O	2.17	0.45
1:A:206:ARG:NH2	3:A:510:HOH:O	2.49	0.45
1:A:301:THR:HA	2:A:403:EDO:H21	1.99	0.45
1:A:122:ALA:HB3	3:A:541:HOH:O	2.17	0.45
1:B:149:LEU:HD13	1:B:161[B]:THR:HG21	1.98	0.45
1:D:152:ASN:HB2	1:D:169:PHE:O	2.16	0.45
1:A:118:GLN:NE2	3:A:511:HOH:O	2.49	0.44
1:D:6:ILE:O	1:D:49:PHE:HA	2.18	0.44
1:B:10:TYR:CZ	1:B:16:GLY:HA3	2.53	0.44
1:B:154:GLN:HE21	1:B:179:VAL:HG11	1.83	0.44
1:A:20:SER:O	1:A:23:GLY:N	2.50	0.44
1:B:14:THR:HA	1:B:17:MET:HG3	2.00	0.44
1:B:95:ALA:HB2	1:B:161[A]:THR:HG23	1.99	0.43
1:D:60:SER:HB2	1:D:89:HIS:CE1	2.53	0.43
1:D:334:LEU:C	1:D:334:LEU:HD12	2.43	0.43
1:D:7:TYR:OH	1:D:74:ASP:OD1	2.32	0.43
1:D:270:LEU:HD23	1:D:297:GLY:HA3	2.00	0.43
1:D:55:ALA:HA	1:D:56:PRO:HA	1.81	0.43
1:D:312:LEU:O	1:D:317:LEU:HD12	2.19	0.43
1:B:55:ALA:HA	1:B:56:PRO:HA	1.81	0.42
1:C:163:LYS:HD2	1:C:171:ALA:O	2.19	0.42
1:C:228:ASN:HB3	1:D:228:ASN:O	2.19	0.42
1:B:88:LEU:HD21	1:B:132:LEU:HD13	2.01	0.42
1:C:199:ASN:N	3:C:510:HOH:O	2.52	0.42
1:C:76:GLN:HB2	1:C:204:VAL:HG21	2.00	0.42
1:B:28:SER:HA	1:B:53:GLU:OE1	2.20	0.41
1:D:252:GLU:HB2	3:D:619:HOH:O	2.20	0.41
1:A:63:MET:HE2	1:A:97:THR:OG1	2.20	0.41
1:C:6:ILE:O	1:C:49:PHE:HA	2.20	0.41
1:C:124:LEU:HG	1:C:125:ARG:HG3	2.03	0.41
1:D:17:MET:HG2	1:D:25:ILE:C	2.46	0.41
1:D:165[A]:HIS:CE1	3:D:583:HOH:O	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:THR:O	1:A:15:ILE:C	2.63	0.41
1:D:121:LEU:CD1	1:D:129:GLN:HA	2.49	0.41
1:A:249:GLN:HG3	1:A:249:GLN:O	2.21	0.40
1:D:57:LEU:HD23	1:D:57:LEU:HA	1.88	0.40
1:A:6:ILE:O	1:A:49:PHE:HA	2.22	0.40
1:B:213:GLY:HA3	3:B:522:HOH:O	2.22	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	321/338 (95%)	313 (98%)	8 (2%)	0	100	100
1	B	308/338 (91%)	301 (98%)	7 (2%)	0	100	100
1	C	305/338 (90%)	296 (97%)	9 (3%)	0	100	100
1	D	297/338 (88%)	285 (96%)	12 (4%)	0	100	100
All	All	1231/1352 (91%)	1195 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	273/283 (96%)	269 (98%)	4 (2%)	57	49
1	B	265/283 (94%)	263 (99%)	2 (1%)	73	70
1	C	265/283 (94%)	261 (98%)	4 (2%)	57	49
1	D	258/283 (91%)	251 (97%)	7 (3%)	39	27
All	All	1061/1132 (94%)	1044 (98%)	17 (2%)	57	47

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	121	LEU
1	A	181	LEU
1	A	316	SER
1	B	161[A]	THR
1	B	161[B]	THR
1	C	2	GLN
1	C	3	LYS
1	C	32	GLN
1	C	121	LEU
1	D	17	MET
1	D	18	GLN
1	D	30	HIS
1	D	59	ASP
1	D	162	THR
1	D	177	LEU
1	D	335	THR

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

Mol	Chain	Res	Type
1	A	18	GLN
1	A	324	GLN
1	A	328	GLN
1	B	18	GLN
1	B	52	HIS
1	B	77	GLN
1	B	134	ASN
1	B	141	ASN
1	B	154	GLN
1	B	246	ASN

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Mol	Chain	Res	Type
1	B	249	GLN
1	B	291	GLN
1	B	315	GLN
1	C	141	ASN
1	C	154	GLN
1	C	246	ASN
1	C	328	GLN
1	D	30	HIS
1	D	145	ASN
1	D	246	ASN
1	D	249	GLN
1	D	328	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	EDO	A	402	-	3,3,3	0.13	0	2,2,2	0.27	0
2	EDO	A	401	-	3,3,3	0.25	0	2,2,2	0.21	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	C	401	-	3,3,3	0.25	0	2,2,2	0.24	0
2	EDO	A	404	-	3,3,3	0.52	0	2,2,2	0.54	0
2	EDO	B	401	-	3,3,3	0.37	0	2,2,2	0.52	0
2	EDO	A	403	-	3,3,3	0.58	0	2,2,2	1.26	0
2	EDO	B	402	-	3,3,3	0.08	0	2,2,2	0.24	0
2	EDO	C	402	-	3,3,3	0.35	0	2,2,2	0.56	0
2	EDO	C	403	-	3,3,3	0.19	0	2,2,2	0.15	0
2	EDO	D	401	-	3,3,3	0.22	0	2,2,2	0.25	0
2	EDO	B	403	-	3,3,3	0.27	0	2,2,2	0.32	0
2	EDO	D	402	-	3,3,3	0.33	0	2,2,2	0.23	0
2	EDO	B	404	-	3,3,3	0.54	0	2,2,2	0.52	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
2	EDO	A	402	-	-	1/1/1/1	-
2	EDO	A	401	-	-	0/1/1/1	-
2	EDO	C	401	-	-	1/1/1/1	-
2	EDO	A	404	-	-	0/1/1/1	-
2	EDO	B	401	-	-	1/1/1/1	-
2	EDO	A	403	-	-	0/1/1/1	-
2	EDO	B	402	-	-	1/1/1/1	-
2	EDO	C	402	-	-	0/1/1/1	-
2	EDO	C	403	-	-	1/1/1/1	-
2	EDO	D	401	-	-	1/1/1/1	-
2	EDO	B	403	-	-	1/1/1/1	-
2	EDO	D	402	-	-	1/1/1/1	-
2	EDO	B	404	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	EDO	O1-C1-C2-O2
2	C	401	EDO	O1-C1-C2-O2
2	C	403	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	B	402	EDO	O1-C1-C2-O2
2	B	403	EDO	O1-C1-C2-O2
2	D	401	EDO	O1-C1-C2-O2
2	B	404	EDO	O1-C1-C2-O2
2	A	402	EDO	O1-C1-C2-O2
2	D	402	EDO	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	EDO	1	0
2	A	404	EDO	2	0
2	B	401	EDO	1	0
2	A	403	EDO	1	0
2	C	402	EDO	1	0
2	C	403	EDO	1	0
2	D	401	EDO	1	0
2	B	403	EDO	3	0
2	B	404	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, 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	319/338 (94%)	0.20	27 (8%) 16 14	9, 26, 53, 78	9 (2%)
1	B	312/338 (92%)	0.49	34 (10%) 10 9	13, 30, 64, 100	5 (1%)
1	C	308/338 (91%)	0.75	40 (12%) 7 6	15, 38, 68, 95	6 (1%)
1	D	303/338 (89%)	1.53	88 (29%) 1 1	28, 56, 83, 99	3 (0%)
All	All	1242/1352 (91%)	0.73	189 (15%) 5 4	9, 37, 73, 100	23 (1%)

All (189) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	169	PHE	8.3
1	D	169	PHE	8.2
1	C	26	PRO	6.2
1	D	25	ILE	6.0
1	A	37	LEU	4.8
1	B	286	GLY	4.5
1	C	183	ALA	4.5
1	C	165[A]	HIS	4.4
1	D	33	ARG	4.3
1	D	18	GLN	4.3
1	C	337	THR	4.2
1	D	144	VAL	4.1
1	D	274	ILE	4.1
1	B	169	PHE	4.1
1	C	181	LEU	3.9
1	B	337	THR	3.9
1	A	337	THR	3.9
1	B	25	ILE	3.9
1	D	30	HIS	3.8
1	C	37	LEU	3.7
1	D	337	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	23	GLY	3.6
1	D	244	VAL	3.6
1	B	124	LEU	3.6
1	D	57	LEU	3.6
1	B	24	TYR	3.6
1	B	183	ALA	3.5
1	D	180	LEU	3.5
1	D	51	ILE	3.5
1	B	181	LEU	3.5
1	D	248	PRO	3.4
1	D	247	ALA	3.4
1	D	249	GLN	3.4
1	C	248	PRO	3.4
1	A	286	GLY	3.3
1	A	20	SER	3.3
1	C	168	GLY	3.3
1	A	24	TYR	3.3
1	B	27	VAL	3.3
1	D	36	ALA	3.3
1	D	55	ALA	3.3
1	D	166	ALA	3.2
1	C	2	GLN	3.2
1	D	118	GLN	3.2
1	A	284	ALA	3.2
1	C	36	ALA	3.2
1	B	42	HIS	3.2
1	C	166	ALA	3.1
1	B	281	GLY	3.1
1	D	37	LEU	3.1
1	B	288	ALA	3.1
1	B	126	SER	3.1
1	B	184	GLY	3.1
1	D	58	ILE	3.0
1	B	206	ARG	3.0
1	C	289	LEU	3.0
1	A	199	ASN	3.0
1	C	55	ALA	3.0
1	D	203	ILE	3.0
1	D	7	TYR	3.0
1	D	278	VAL	3.0
1	C	245	GLY	3.0
1	B	180	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	81	LEU	2.9
1	A	118	GLN	2.9
1	C	118	GLN	2.9
1	A	36	ALA	2.9
1	D	15	ILE	2.9
1	D	121	LEU	2.9
1	A	184	GLY	2.9
1	A	169	PHE	2.9
1	D	17	MET	2.9
1	D	179	VAL	2.9
1	D	204	VAL	2.9
1	C	244	VAL	2.8
1	D	26	PRO	2.8
1	D	49	PHE	2.8
1	D	168	GLY	2.8
1	D	109	ALA	2.8
1	D	171	ALA	2.8
1	D	246	ASN	2.8
1	B	249	GLN	2.8
1	C	253	LEU	2.8
1	D	27	VAL	2.8
1	C	170	ASP	2.8
1	A	126	SER	2.8
1	D	122	ALA	2.8
1	B	19	ARG	2.8
1	B	200	GLY	2.8
1	D	119	ILE	2.8
1	A	124	LEU	2.7
1	C	122	ALA	2.7
1	C	251	ALA	2.7
1	D	271	THR	2.7
1	B	26	PRO	2.7
1	B	201	PRO	2.7
1	B	118	GLN	2.7
1	B	125	ARG	2.7
1	D	82	TYR	2.7
1	D	200	GLY	2.7
1	D	277	SER	2.7
1	C	164	ALA	2.6
1	D	31	LEU	2.6
1	D	202	LEU	2.6
1	B	141	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	47	PRO	2.6
1	A	19	ARG	2.6
1	C	278	VAL	2.6
1	D	10	TYR	2.6
1	D	56	PRO	2.6
1	D	77	GLN	2.6
1	D	4	LYS	2.6
1	A	27	VAL	2.6
1	A	285	THR	2.6
1	D	245	GLY	2.5
1	D	251	ALA	2.5
1	C	27	VAL	2.5
1	D	8	VAL	2.5
1	D	50	THR	2.5
1	B	32	GLN	2.5
1	C	180	LEU	2.5
1	C	274	ILE	2.5
1	D	316	SER	2.5
1	D	177	LEU	2.5
1	D	330	LEU	2.4
1	A	249	GLN	2.4
1	B	51	ILE	2.4
1	A	122	ALA	2.4
1	A	31	LEU	2.4
1	D	63	MET	2.4
1	D	143	PRO	2.4
1	D	142	HIS	2.4
1	D	273	SER	2.4
1	D	6	ILE	2.4
1	D	75	ILE	2.4
1	C	290	ALA	2.4
1	D	70	HIS	2.4
1	C	273	SER	2.4
1	D	250	LYS	2.4
1	C	254	LEU	2.3
1	D	137	TYR	2.3
1	B	122	ALA	2.3
1	C	15	ILE	2.3
1	B	182	GLU	2.3
1	D	42	HIS	2.3
1	D	52	HIS	2.3
1	B	17	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	63	MET	2.3
1	B	29	GLY	2.3
1	D	35	LEU	2.3
1	D	105	LEU	2.3
1	D	207	ILE	2.3
1	D	240	ARG	2.3
1	B	144	VAL	2.3
1	D	108	LEU	2.3
1	C	242	TYR	2.2
1	D	79	TYR	2.2
1	D	201	PRO	2.2
1	C	246	ASN	2.2
1	D	252	GLU	2.2
1	A	26	PRO	2.2
1	C	277	SER	2.2
1	D	16	GLY	2.2
1	D	213	GLY	2.2
1	D	242	TYR	2.2
1	C	58	ILE	2.2
1	C	17	MET	2.2
1	B	37	LEU	2.2
1	C	249	GLN	2.2
1	D	313	LEU	2.2
1	A	283	TYR	2.2
1	C	287	ASN	2.2
1	D	253	LEU	2.2
1	D	28	SER	2.1
1	D	275	SER	2.1
1	A	282	GLY	2.1
1	A	182	GLU	2.1
1	D	41	PHE	2.1
1	B	119	ILE	2.1
1	D	62	ASP	2.1
1	C	243	GLY	2.1
1	D	45	GLU	2.1
1	D	133	LEU	2.1
1	A	183	ALA	2.1
1	A	119	ILE	2.0
1	A	316	SER	2.0
1	C	217	ILE	2.0
1	D	139	ALA	2.0
1	B	205	HIS	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 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($\text{\AA}^2$)	Q<0.9
2	EDO	C	401	4/4	0.77	0.23	57,69,69,70	0
2	EDO	A	404	4/4	0.81	0.19	48,56,57,64	0
2	EDO	A	402	4/4	0.82	0.15	49,49,50,55	0
2	EDO	C	403	4/4	0.83	0.24	51,57,63,75	0
2	EDO	D	402	4/4	0.83	0.18	46,47,51,53	0
2	EDO	A	401	4/4	0.85	0.16	42,54,54,64	0
2	EDO	B	403	4/4	0.86	0.16	47,52,55,57	0
2	EDO	B	401	4/4	0.87	0.19	32,39,44,63	0
2	EDO	B	402	4/4	0.88	0.14	56,59,62,69	0
2	EDO	D	401	4/4	0.89	0.15	54,59,62,62	0
2	EDO	C	402	4/4	0.90	0.16	54,54,55,56	0
2	EDO	B	404	4/4	0.90	0.18	34,42,44,45	0
2	EDO	A	403	4/4	0.93	0.13	33,36,42,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.