



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 05:27 PM UTC

PDB ID : 7R6B / pdb_00007r6b
Title : Crystal structure of mutant R43D/L124D/R125A/C273S of L-Asparaginase I from *Yersinia pestis*
Authors : Strzelczyk, P.; Wlodawer, A.; Lubkowski, J.
Deposited on : 2021-06-22
Resolution : 2.03 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

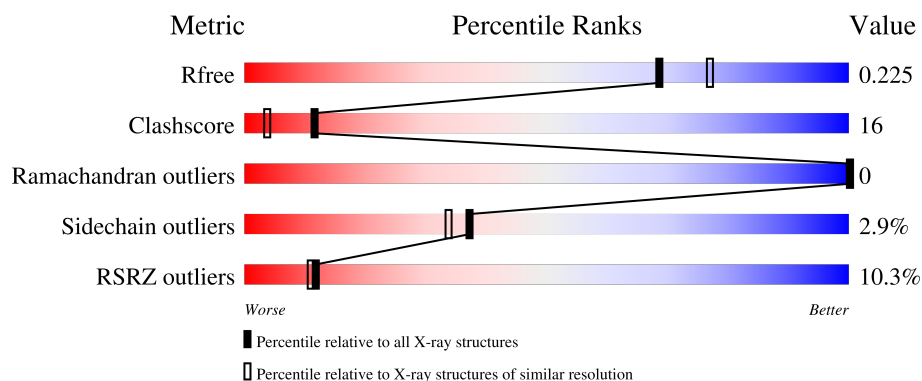
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.03 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	9% 68% 19% • 11%
1	B	338	9% 65% 21% • 11%

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	EDO	A	401	-	-	X	-
2	EDO	B	406	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5099 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	302	Total	C	N	O	S	0	3	0
			2342	1486	397	450	9			
1	B	301	Total	C	N	O	S	0	3	0
			2332	1484	396	443	9			

There are 10 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	124	ASP	LEU	engineered mutation	UNP A0A3N4B0Q2
A	125	ALA	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	124	ASP	LEU	engineered mutation	UNP A0A3N4B0Q2
B	125	ALA	ARG	engineered mutation	UNP A0A3N4B0Q2
B	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 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Ca 2 2	0	0

- Molecule 4 is water.

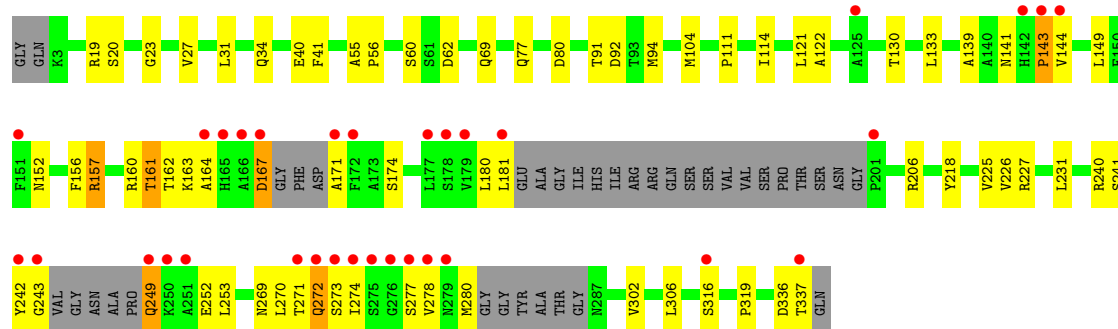
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	180	Total 180	O 180	0	0
4	B	203	Total 203	O 203	0	0

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.

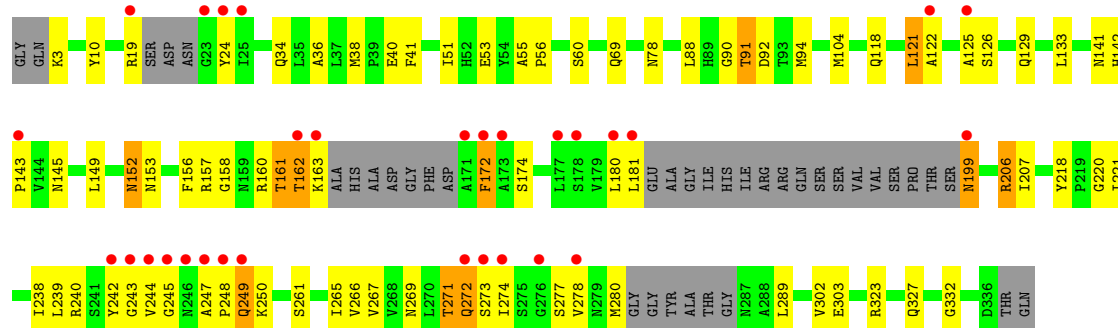
• Molecule 1: L-asparaginase I

Chain A: 



• Molecule 1: L-asparaginase I

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	100.26Å 115.89Å 127.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.85 – 2.03 48.85 – 2.03	Depositor EDS
% Data completeness (in resolution range)	96.2 (48.85-2.03) 96.4 (48.85-2.03)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.170 , 0.218 0.181 , 0.225	Depositor DCC
R_{free} test set	2372 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.2	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	0.95	EDS
Total number of atoms	5099	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	1.28	6/2397 (0.3%)	1.45	14/3258 (0.4%)
1	B	1.30	6/2383 (0.3%)	1.47	13/3240 (0.4%)
All	All	1.29	12/4780 (0.3%)	1.46	27/6498 (0.4%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	206	ARG	C-N	-7.26	1.24	1.33
1	A	31	LEU	C-O	6.71	1.31	1.24
1	B	238	ILE	C-O	6.52	1.31	1.24
1	A	161	THR	C-O	6.46	1.31	1.23
1	B	161	THR	C-O	6.42	1.31	1.23
1	B	90	GLY	C-O	5.66	1.29	1.23
1	A	143	PRO	N-CA	-5.41	1.40	1.47
1	A	231	LEU	C-O	5.29	1.31	1.23
1	B	277	SER	C-O	5.17	1.30	1.23
1	A	80	ASP	C-O	-5.10	1.17	1.24
1	B	327	GLN	C-O	-5.01	1.17	1.24
1	A	225	VAL	C-O	5.00	1.29	1.24

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	249	GLN	N-CA-C	-7.47	103.06	113.37
1	B	121	LEU	CA-C-N	6.96	129.94	120.54
1	B	121	LEU	C-N-CA	6.96	129.94	120.54
1	B	152	ASN	CB-CA-C	-6.19	102.76	111.80
1	A	144	VAL	N-CA-C	-6.17	98.99	107.99
1	A	157	ARG	CA-C-N	5.73	126.46	119.99
1	A	157	ARG	C-N-CA	5.73	126.46	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ASN	CA-C-N	-5.70	115.99	123.34
1	A	141	ASN	C-N-CA	-5.70	115.99	123.34
1	B	239	LEU	N-CA-CB	-5.57	101.34	110.42
1	A	206	ARG	N-CA-CB	-5.47	101.97	110.29
1	A	241	SER	CA-C-N	5.42	128.53	120.95
1	A	241	SER	C-N-CA	5.42	128.53	120.95
1	A	130	THR	N-CA-C	-5.33	105.55	111.36
1	A	19	ARG	CB-CA-C	5.33	118.21	109.90
1	A	272	GLN	CA-C-N	5.30	131.07	122.53
1	A	272	GLN	C-N-CA	5.30	131.07	122.53
1	B	172	PHE	CA-CB-CG	-5.26	108.53	113.80
1	B	158	GLY	CA-C-O	-5.20	115.70	121.05
1	B	78	ASN	CA-CB-CG	-5.16	107.44	112.60
1	B	53	GLU	CB-CA-C	5.11	118.75	110.22
1	B	91	THR	CA-CB-OG1	-5.07	101.99	109.60
1	A	277	SER	CA-C-N	5.07	127.87	120.98
1	A	277	SER	C-N-CA	5.07	127.87	120.98
1	B	271	THR	CA-C-O	-5.07	115.16	120.58
1	B	277	SER	CA-C-N	5.04	127.34	120.63
1	B	277	SER	C-N-CA	5.04	127.34	120.63

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	2342	0	2324	65	0
1	B	2332	0	2329	91	0
2	A	16	0	24	8	0
2	B	24	0	36	16	0
3	B	2	0	0	0	0
4	A	180	0	0	10	0
4	B	203	0	0	6	0
All	All	5099	0	4713	151	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 16.

All (151) 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:A:111:PRO:HG3	1:A:143:PRO:HB3	1.35	1.08
1:B:271:THR:HG23	1:B:278:VAL:HG22	1.34	1.08
1:B:34[B]:GLN:HE22	1:B:122:ALA:HB2	1.14	1.07
1:B:243:GLY:O	1:B:271:THR:HB	1.56	1.04
1:B:34[B]:GLN:HE22	1:B:122:ALA:CB	1.74	0.99
1:A:240:ARG:HB3	1:A:272:GLN:CB	1.96	0.96
1:B:245:GLY:HA2	1:B:271:THR:HG22	1.53	0.90
1:A:271:THR:H	1:A:278:VAL:HG22	1.41	0.86
1:B:34[B]:GLN:NE2	1:B:122:ALA:HB2	1.90	0.85
1:B:323:ARG:HE	2:B:406:EDO:C1	1.89	0.85
1:A:240:ARG:HE	1:A:272:GLN:HG2	1.41	0.84
1:B:141:ASN:C	1:B:143:PRO:HD3	2.01	0.83
1:A:40:GLU:HG3	4:A:563:HOH:O	1.78	0.82
1:B:323:ARG:HE	2:B:406:EDO:H12	1.43	0.82
1:B:91:THR:HA	1:B:94:MET:HE3	1.62	0.81
1:B:271:THR:HG23	1:B:278:VAL:CG2	2.10	0.81
1:A:91:THR:HA	1:A:94:MET:HE3	1.61	0.81
1:A:240:ARG:HB3	1:A:272:GLN:HB3	1.65	0.78
1:A:271:THR:H	1:A:278:VAL:CG2	1.98	0.76
1:A:271:THR:N	1:A:278:VAL:HG22	2.00	0.75
1:B:271:THR:CG2	1:B:278:VAL:HG22	2.16	0.72
1:A:240:ARG:HE	1:A:272:GLN:CG	2.03	0.72
1:B:240:ARG:HB3	1:B:272:GLN:HG2	1.71	0.71
1:B:261:SER:HB2	2:B:406:EDO:O2	1.90	0.71
1:B:265:ILE:O	2:B:406:EDO:H21	1.91	0.71
1:B:125:ALA:C	4:B:502:HOH:O	2.33	0.71
1:B:271:THR:HG21	1:B:278:VAL:HA	1.72	0.70
1:B:126:SER:N	4:B:502:HOH:O	2.23	0.70
1:B:245:GLY:CA	1:B:271:THR:HG22	2.21	0.70
1:A:240:ARG:NE	1:A:272:GLN:HG2	2.07	0.70
1:A:243:GLY:O	1:A:271:THR:HG21	1.92	0.69
1:B:142:HIS:N	1:B:143:PRO:HD3	2.08	0.68
1:A:249:GLN:N	4:A:503:HOH:O	2.27	0.68
1:B:34[B]:GLN:HE22	1:B:122:ALA:CA	2.07	0.68
1:A:337:THR:C	4:A:512:HOH:O	2.35	0.67
1:B:240:ARG:HB3	1:B:272:GLN:CG	2.25	0.67
1:A:240:ARG:HB3	1:A:272:GLN:HB2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:34[B]:GLN:NE2	1:B:122:ALA:CB	2.54	0.66
1:A:181:LEU:C	1:A:181:LEU:HD23	2.22	0.65
1:B:69:GLN:HA	1:B:104:MET:HE1	1.78	0.65
1:B:248:PRO:C	1:B:250:LYS:H	2.03	0.65
1:B:157:ARG:O	1:B:161:THR:HG23	1.98	0.63
1:A:62:ASP:HA	1:B:248:PRO:HB3	1.78	0.63
1:B:152:ASN:HD21	1:B:172:PHE:H	1.43	0.63
1:A:111:PRO:HG3	1:A:143:PRO:CB	2.23	0.63
1:A:156:PHE:HB3	1:A:161:THR:HG22	1.80	0.62
1:B:156:PHE:HB3	1:B:161:THR:HG22	1.82	0.62
2:A:403:EDO:H12	4:A:664:HOH:O	2.00	0.61
1:B:267:VAL:H	2:B:406:EDO:C2	2.13	0.60
1:B:245:GLY:N	1:B:271:THR:CG2	2.64	0.60
1:A:227:ARG:HG2	2:A:401:EDO:H12	1.83	0.60
1:B:245:GLY:HA2	1:B:271:THR:CG2	2.31	0.60
1:A:240:ARG:HE	1:A:272:GLN:CD	2.09	0.60
1:A:157:ARG:O	1:A:161:THR:HG23	2.02	0.59
1:B:240:ARG:CZ	1:B:302[A]:VAL:HG21	2.32	0.59
1:A:271:THR:OG1	1:A:278:VAL:HG22	2.02	0.59
1:B:245:GLY:N	1:B:271:THR:HG21	2.18	0.58
1:A:227:ARG:HD3	2:A:401:EDO:H11	1.85	0.58
1:A:111:PRO:CG	1:A:143:PRO:HB3	2.24	0.57
1:B:34[A]:GLN:HE21	1:B:38:MET:HE3	1.68	0.57
1:B:271:THR:CG2	1:B:278:VAL:HA	2.34	0.56
1:B:160:ARG:O	1:B:174:SER:HA	2.06	0.56
1:A:34[B]:GLN:NE2	1:A:122:ALA:HB2	2.21	0.55
1:B:248:PRO:C	1:B:250:LYS:N	2.64	0.55
1:A:77:GLN:HG3	4:A:521:HOH:O	2.06	0.55
1:B:245:GLY:CA	1:B:271:THR:CG2	2.85	0.55
1:A:227:ARG:CD	2:A:401:EDO:H11	2.38	0.54
1:B:271:THR:N	1:B:278:VAL:HG22	2.22	0.54
1:A:160:ARG:O	1:A:174:SER:HA	2.07	0.54
1:B:156:PHE:CB	1:B:161:THR:HG22	2.38	0.54
1:B:261:SER:CB	2:B:406:EDO:O2	2.56	0.53
1:A:240:ARG:CB	1:A:272:GLN:HB2	2.38	0.53
1:A:227:ARG:HG2	2:A:401:EDO:C1	2.39	0.53
1:B:323:ARG:NE	2:B:406:EDO:H12	2.19	0.53
1:A:243:GLY:O	1:A:271:THR:CG2	2.57	0.53
1:B:244:VAL:C	1:B:271:THR:HG21	2.33	0.52
1:A:149:LEU:C	1:A:149:LEU:HD23	2.34	0.52
1:A:278:VAL:HG12	1:A:280:MET:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ARG:NH1	1:A:252:GLU:OE1	2.43	0.52
1:A:167:ASP:C	1:A:167:ASP:OD2	2.53	0.52
1:A:69:GLN:HA	1:A:104:MET:HE1	1.90	0.52
1:A:218:TYR:C	1:A:242:TYR:OH	2.53	0.51
1:A:60:SER:OG	1:A:92:ASP:OD1	2.22	0.51
1:A:111:PRO:HG2	1:A:139:ALA:O	2.10	0.51
1:B:104:MET:HG2	1:B:207[A]:ILE:HG13	1.93	0.51
1:B:143:PRO:HB2	2:B:405:EDO:H21	1.92	0.51
1:B:180:LEU:C	1:B:181:LEU:HG	2.36	0.51
1:A:27:VAL:HG11	2:A:404:EDO:H12	1.93	0.50
1:A:226:VAL:HG21	1:A:253:LEU:HD13	1.93	0.50
1:B:10:TYR:HA	1:B:88:LEU:HB2	1.93	0.50
1:B:266:VAL:HA	2:B:406:EDO:H12	1.95	0.49
1:B:248:PRO:HB2	1:B:250:LYS:H	1.76	0.49
1:B:247:ALA:HB3	1:B:289:LEU:HD21	1.94	0.49
4:A:631:HOH:O	1:B:249:GLN:HB2	2.13	0.48
1:B:38:MET:HE1	1:B:121:LEU:CD2	2.43	0.48
1:A:273:SER:OG	1:B:163:LYS:HG2	2.13	0.48
1:B:149:LEU:C	1:B:149:LEU:HD23	2.38	0.48
1:B:269:ASN:OD1	1:B:280:MET:HE3	2.13	0.48
1:B:271:THR:HG23	1:B:278:VAL:CB	2.43	0.48
1:B:36:ALA:HB1	2:B:401:EDO:H22	1.96	0.48
1:B:143:PRO:HG2	2:B:405:EDO:H11	1.96	0.48
1:A:269:ASN:O	1:A:278:VAL:HG21	2.14	0.47
1:B:142:HIS:N	1:B:143:PRO:CD	2.77	0.47
1:A:20:SER:OG	1:A:23:GLY:O	2.28	0.47
1:B:245:GLY:N	1:B:271:THR:HG22	2.30	0.47
1:B:248:PRO:HB2	1:B:250:LYS:CB	2.45	0.47
1:A:156:PHE:CB	1:A:161:THR:HG22	2.45	0.46
1:B:118:GLN:HG2	4:B:507:HOH:O	2.15	0.46
1:A:163:LYS:HD2	1:A:171:ALA:O	2.16	0.46
1:A:41:PHE:CZ	1:A:133:LEU:HG	2.51	0.46
1:A:336:ASP:HA	4:A:648:HOH:O	2.16	0.46
1:B:267:VAL:H	2:B:406:EDO:C1	2.30	0.45
1:A:271:THR:OG1	1:A:278:VAL:HA	2.17	0.45
1:A:274:ILE:HG23	1:B:274:ILE:HD12	1.99	0.45
1:B:55:ALA:HA	1:B:56:PRO:HA	1.83	0.45
1:B:162:THR:HA	1:B:303:GLU:OE2	2.16	0.44
1:A:164:ALA:HA	1:B:274:ILE:HG12	1.99	0.44
1:B:69:GLN:OE1	1:B:206:ARG:HD2	2.18	0.44
1:A:240:ARG:CZ	1:A:302[A]:VAL:HG21	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:TYR:HB3	1:B:92:ASP:HB2	1.99	0.44
1:B:38:MET:HE1	1:B:121:LEU:HD23	1.99	0.44
1:B:38:MET:SD	1:B:129:GLN:NE2	2.90	0.44
1:B:41:PHE:CZ	1:B:133:LEU:HG	2.53	0.44
1:A:34[A]:GLN:NE2	4:A:506:HOH:O	2.32	0.44
1:B:332:GLY:HA2	4:B:619:HOH:O	2.17	0.43
1:A:180:LEU:HD11	4:A:545:HOH:O	2.17	0.43
1:A:306:LEU:C	1:A:306:LEU:HD13	2.43	0.43
1:B:206:ARG:HB3	4:B:645:HOH:O	2.18	0.43
1:A:55:ALA:HA	1:A:56:PRO:HA	1.89	0.43
1:A:227:ARG:CD	2:A:401:EDO:C1	2.96	0.43
1:A:92:ASP:HB2	1:B:242:TYR:HB3	2.00	0.43
1:B:34[B]:GLN:NE2	1:B:122:ALA:CA	2.79	0.43
1:A:242:TYR:HD1	2:A:403:EDO:H22	1.84	0.42
1:B:60:SER:OG	1:B:92:ASP:OD1	2.24	0.42
1:A:240:ARG:HB3	1:A:272:GLN:CG	2.47	0.42
1:B:323:ARG:NE	2:B:406:EDO:C1	2.71	0.42
1:B:19:ARG:HG3	1:B:24:TYR:CE1	2.54	0.42
1:B:91:THR:HA	1:B:94:MET:CE	2.43	0.42
1:A:270:LEU:O	1:A:272:GLN:N	2.53	0.42
1:B:269:ASN:OD1	1:B:280:MET:CE	2.68	0.41
4:A:631:HOH:O	1:B:249:GLN:CB	2.68	0.41
1:B:218:TYR:C	1:B:242:TYR:OH	2.64	0.41
1:B:323:ARG:HH21	2:B:406:EDO:H12	1.86	0.41
1:A:152:ASN:OD1	1:A:171:ALA:N	2.53	0.41
1:B:145:ASN:HD21	2:B:405:EDO:C2	2.33	0.41
1:B:160:ARG:HB3	1:B:174:SER:HB2	2.03	0.41
1:B:323:ARG:HE	2:B:406:EDO:H11	1.82	0.41
1:B:220:GLY:O	1:B:221:ILE:C	2.61	0.41
1:A:160:ARG:HB3	1:A:174:SER:HB2	2.02	0.40
1:B:34[B]:GLN:NE2	1:B:122:ALA:HA	2.36	0.40
1:B:199:ASN:HB3	4:B:514:HOH:O	2.20	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	295/338 (87%)	286 (97%)	9 (3%)	0	100	100
1	B	294/338 (87%)	288 (98%)	6 (2%)	0	100	100
All	All	589/676 (87%)	574 (98%)	15 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	260/282 (92%)	253 (97%)	7 (3%)	39	37
1	B	258/282 (92%)	250 (97%)	8 (3%)	35	31
All	All	518/564 (92%)	503 (97%)	15 (3%)	37	34

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	ILE
1	A	121	LEU
1	A	162	THR
1	A	167	ASP
1	A	249	GLN
1	A	316	SER
1	A	319	PRO
1	B	3	LYS
1	B	40	GLU
1	B	51	ILE
1	B	153	ASN
1	B	162	THR
1	B	199	ASN
1	B	272	GLN

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Mol	Chain	Res	Type
1	B	273	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	129	GLN
1	A	134	ASN
1	A	152	ASN
1	A	153	ASN
1	A	165	HIS
1	A	249	GLN
1	A	269	ASN
1	B	18	GLN
1	B	42	HIS
1	B	129	GLN
1	B	134	ASN
1	B	145	ASN
1	B	152	ASN
1	B	249	GLN
1	B	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](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EDO	A	404	-	3,3,3	0.29	0	2,2,2	0.12	0
2	EDO	B	404	-	3,3,3	0.26	0	2,2,2	0.59	0
2	EDO	A	403	-	3,3,3	0.31	0	2,2,2	0.17	0
2	EDO	B	403	-	3,3,3	0.16	0	2,2,2	0.36	0
2	EDO	B	401	-	3,3,3	0.18	0	2,2,2	0.39	0
2	EDO	B	406	-	3,3,3	0.65	0	2,2,2	1.04	0
2	EDO	B	402	-	3,3,3	0.18	0	2,2,2	0.33	0
2	EDO	B	405	-	3,3,3	0.34	0	2,2,2	0.14	0
2	EDO	A	401	-	3,3,3	0.16	0	2,2,2	0.32	0
2	EDO	A	402	-	3,3,3	0.13	0	2,2,2	0.39	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	404	-	-	1/1/1/1	-
2	EDO	B	404	-	-	0/1/1/1	-
2	EDO	A	403	-	-	1/1/1/1	-
2	EDO	B	403	-	-	1/1/1/1	-
2	EDO	B	401	-	-	1/1/1/1	-
2	EDO	B	406	-	-	1/1/1/1	-
2	EDO	B	402	-	-	0/1/1/1	-
2	EDO	B	405	-	-	1/1/1/1	-
2	EDO	A	401	-	-	0/1/1/1	-
2	EDO	A	402	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	401	EDO	O1-C1-C2-O2
2	A	403	EDO	O1-C1-C2-O2
2	A	404	EDO	O1-C1-C2-O2
2	B	406	EDO	O1-C1-C2-O2
2	B	403	EDO	O1-C1-C2-O2
2	B	405	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	404	EDO	1	0
2	A	403	EDO	2	0
2	B	401	EDO	1	0
2	B	406	EDO	12	0
2	B	405	EDO	3	0
2	A	401	EDO	5	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	302/338 (89%)	0.26	32 (10%)	11 10	13, 27, 70, 100	3 (0%)
1	B	301/338 (89%)	0.28	30 (9%)	12 11	9, 29, 66, 90	3 (0%)
All	All	603/676 (89%)	0.27	62 (10%)	12 11	9, 28, 68, 100	6 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	248	PRO	5.8
1	A	278	VAL	5.2
1	B	244	VAL	5.0
1	A	181	LEU	4.9
1	B	274	ILE	4.7
1	A	164	ALA	4.5
1	A	242	TYR	4.3
1	A	272	GLN	4.3
1	B	245	GLY	4.1
1	A	243	GLY	4.0
1	A	201	PRO	4.0
1	B	172	PHE	3.8
1	B	199	ASN	3.7
1	A	250	LYS	3.7
1	A	172	PHE	3.7
1	B	242	TYR	3.6
1	B	171	ALA	3.5
1	B	243	GLY	3.4
1	B	273	SER	3.4
1	A	274	ILE	3.4
1	B	247	ALA	3.4
1	B	181	LEU	3.4
1	A	337	THR	3.4
1	B	249	GLN	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	166	ALA	3.2
1	A	143	PRO	3.1
1	B	122	ALA	3.1
1	B	163	LYS	3.0
1	A	171	ALA	2.9
1	B	246	ASN	2.9
1	B	23	GLY	2.9
1	A	249	GLN	2.9
1	A	151	PHE	2.8
1	B	178	SER	2.8
1	A	276	GLY	2.8
1	A	251	ALA	2.7
1	A	144	VAL	2.7
1	B	125	ALA	2.7
1	B	177	LEU	2.7
1	B	24	TYR	2.7
1	B	272	GLN	2.7
1	A	277	SER	2.7
1	A	167	ASP	2.6
1	B	278	VAL	2.6
1	A	273	SER	2.6
1	A	271	THR	2.5
1	A	142	HIS	2.5
1	B	19	ARG	2.5
1	A	178	SER	2.4
1	A	275	SER	2.4
1	B	25	ILE	2.3
1	A	177	LEU	2.3
1	B	180	LEU	2.3
1	B	173	ALA	2.3
1	A	165	HIS	2.2
1	A	316	SER	2.2
1	A	179	VAL	2.2
1	A	279	ASN	2.2
1	A	125	ALA	2.1
1	B	162	THR	2.1
1	B	276	GLY	2.1
1	B	143	PRO	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
2	EDO	B	405	4/4	0.69	0.19	54,60,64,67	0
2	EDO	A	402	4/4	0.72	0.19	47,56,57,57	0
2	EDO	B	403	4/4	0.75	0.17	52,58,61,67	0
2	EDO	B	404	4/4	0.80	0.22	34,45,49,63	0
2	EDO	A	404	4/4	0.80	0.15	60,63,63,64	0
2	EDO	A	403	4/4	0.82	0.16	34,42,43,45	0
2	EDO	B	401	4/4	0.84	0.17	56,58,63,65	0
2	EDO	A	401	4/4	0.86	0.14	58,60,63,70	0
2	EDO	B	402	4/4	0.87	0.16	62,67,68,73	0
3	CA	B	408	1/1	0.89	0.12	66,66,66,66	0
2	EDO	B	406	4/4	0.94	0.18	24,27,32,33	0
3	CA	B	407	1/1	0.98	0.07	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.