



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:51 AM UTC

PDB ID : 7R6A / pdb_00007r6a
Title : Crystal structure of mutant L124D/R125A/C273S of L-Asparaginase I from *Yersinia pestis*
Authors : Strzelczyk, P.; Wlodawer, A.; Lubkowski, J.
Deposited on : 2021-06-22
Resolution : 1.89 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

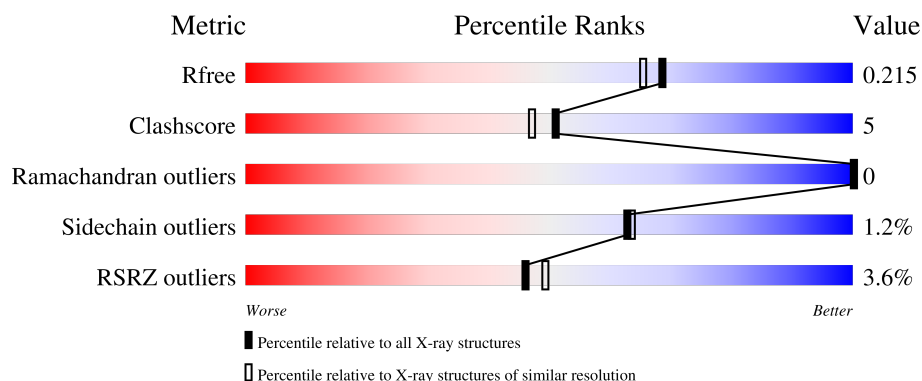
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	4% 83% 13% ..
1	B	338	6% 83% 12% 5%
1	C	338	3% 79% 13% 6%
1	D	338	% 86% 8% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11403 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.

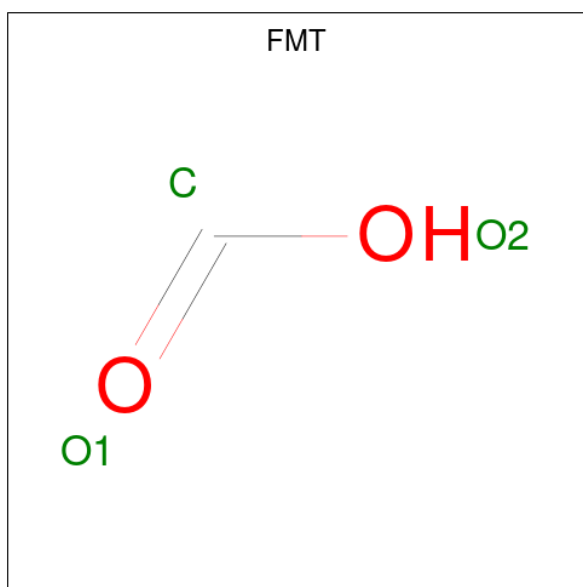
- Molecule 1 is a protein called L-asparaginase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	4	0
			2531	1603	433	486	9			
1	B	322	Total	C	N	O	S	0	9	0
			2510	1590	428	483	9			
1	C	317	Total	C	N	O	S	0	5	0
			2456	1560	419	468	9			
1	D	323	Total	C	N	O	S	0	7	0
			2508	1592	427	480	9			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	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	124	ASP	LEU	engineered mutation	UNP A0A3N4B0Q2
B	125	ALA	ARG	engineered mutation	UNP A0A3N4B0Q2
B	273	SER	CYS	engineered mutation	UNP A0A3N4B0Q2
C	1	GLY	-	expression tag	UNP A0A3N4B0Q2
C	124	ASP	LEU	engineered mutation	UNP A0A3N4B0Q2
C	125	ALA	ARG	engineered mutation	UNP A0A3N4B0Q2
C	273	SER	CYS	engineered mutation	UNP A0A3N4B0Q2
D	1	GLY	-	expression tag	UNP A0A3N4B0Q2
D	124	ASP	LEU	engineered mutation	UNP A0A3N4B0Q2
D	125	ALA	ARG	engineered mutation	UNP A0A3N4B0Q2
D	273	SER	CYS	engineered mutation	UNP A0A3N4B0Q2

- Molecule 2 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	373	Total	O	0	0
			373	373		
3	B	360	Total	O	0	0
			360	360		

Continued on next page...

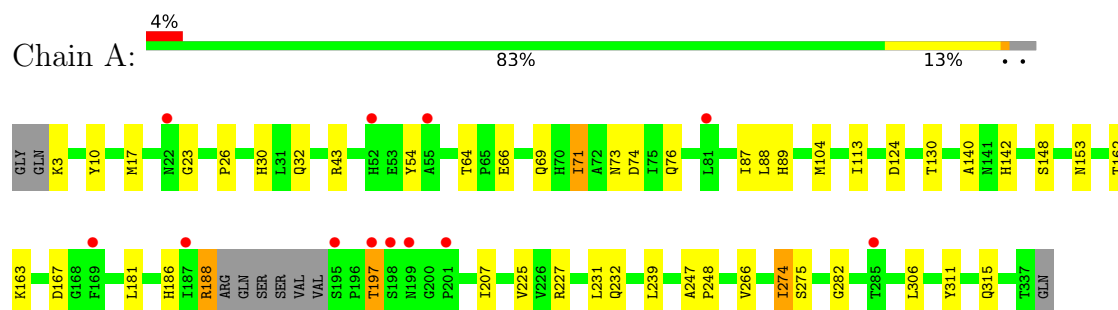
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	307	Total 307	O 307	0	0
3	D	328	Total 328	O 328	0	0

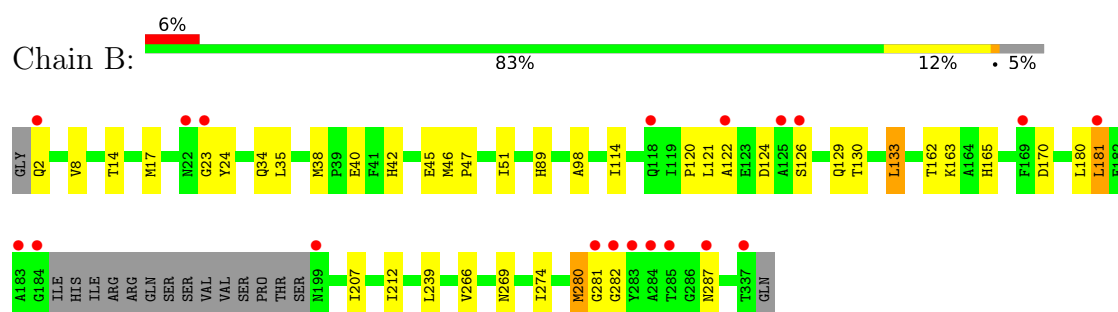
3 Residue-property plots [i](#)

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.

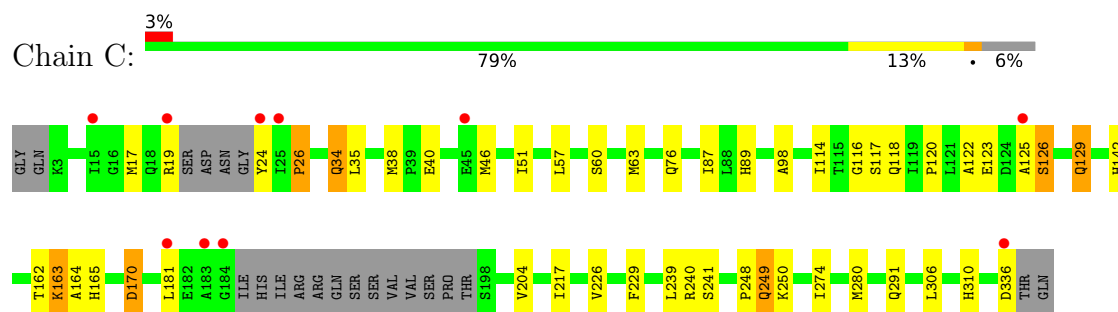
• Molecule 1: L-asparaginase I



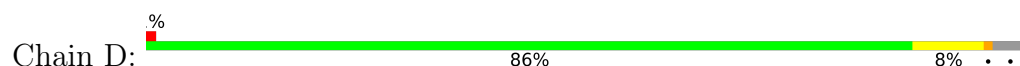
• Molecule 1: L-asparaginase I

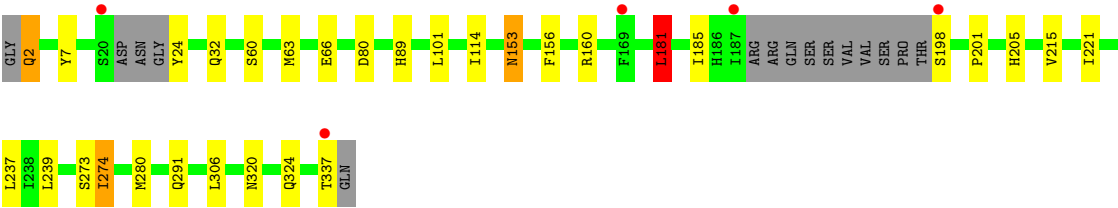


• Molecule 1: L-asparaginase I



• Molecule 1: L-asparaginase I





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.12Å 98.91Å 180.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.88 – 1.89 40.88 – 1.89	Depositor EDS
% Data completeness (in resolution range)	97.7 (40.88-1.89) 98.0 (40.88-1.89)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.157 , 0.211 0.169 , 0.215	Depositor DCC
R_{free} test set	2161 reflections (1.89%)	wwPDB-VP
Wilson B-factor (Å ²)	19.5	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11403	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.20% 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: FMT

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	1.35	14/2594 (0.5%)	1.36	10/3531 (0.3%)
1	B	1.37	7/2584 (0.3%)	1.36	13/3516 (0.4%)
1	C	1.31	10/2516 (0.4%)	1.38	15/3421 (0.4%)
1	D	1.36	8/2578 (0.3%)	1.36	11/3507 (0.3%)
All	All	1.35	39/10272 (0.4%)	1.37	49/13975 (0.4%)

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	117	SER	C-O	-7.98	1.14	1.23
1	B	47	PRO	C-O	7.48	1.32	1.23
1	A	30	HIS	CE1-NE2	7.40	1.40	1.32
1	D	205	HIS	CE1-NE2	7.37	1.40	1.32
1	B	266	VAL	C-O	7.35	1.31	1.23
1	D	89	HIS	CE1-NE2	7.29	1.39	1.32
1	B	181	LEU	C-O	7.14	1.32	1.23
1	C	310	HIS	CE1-NE2	7.01	1.39	1.32
1	A	54	TYR	C-O	7.00	1.32	1.23
1	B	212	ILE	C-O	6.47	1.30	1.24
1	C	126	SER	C-O	6.45	1.31	1.24
1	B	126	SER	C-O	6.41	1.31	1.23
1	A	142	HIS	CE1-NE2	6.31	1.38	1.32
1	A	186	HIS	C-O	6.30	1.31	1.23
1	C	181	LEU	C-O	6.10	1.31	1.23
1	A	197	THR	C-O	5.89	1.30	1.23
1	B	282	GLY	C-O	5.87	1.30	1.23
1	A	167	ASP	C-O	5.84	1.30	1.23
1	D	221	ILE	C-O	5.81	1.29	1.24
1	D	273	SER	C-O	-5.80	1.16	1.23
1	C	26	PRO	C-O	-5.75	1.17	1.23
1	A	282	GLY	C-O	5.68	1.30	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	87	ILE	C-O	5.68	1.30	1.24
1	C	280	MET	C-O	5.59	1.30	1.24
1	A	71	ILE	C-O	5.48	1.30	1.24
1	A	64	THR	N-CA	5.45	1.49	1.46
1	C	204	VAL	C-O	-5.42	1.18	1.24
1	D	237	LEU	C-O	5.37	1.30	1.24
1	A	266	VAL	C-O	5.37	1.30	1.23
1	D	185	ILE	C-O	5.37	1.29	1.24
1	D	160	ARG	C-O	5.36	1.31	1.24
1	C	76	GLN	C-O	-5.27	1.18	1.24
1	A	26	PRO	C-O	-5.23	1.18	1.23
1	A	163	LYS	C-O	-5.21	1.17	1.23
1	A	124	ASP	C-O	-5.15	1.18	1.24
1	B	281	GLY	C-O	5.03	1.28	1.23
1	A	225	VAL	C-O	5.02	1.29	1.24
1	C	142	HIS	CE1-NE2	5.01	1.37	1.32
1	D	156	PHE	C-O	5.00	1.29	1.23

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	274	ILE	N-CA-CB	-7.64	102.03	110.51
1	A	89	HIS	CA-CB-CG	7.43	121.23	113.80
1	A	66	GLU	CB-CG-CD	6.76	124.10	112.60
1	A	74	ASP	CA-CB-CG	6.51	119.11	112.60
1	C	249	GLN	CA-C-N	6.48	133.92	121.54
1	C	249	GLN	C-N-CA	6.48	133.92	121.54
1	A	197	THR	CA-CB-OG1	-6.25	100.22	109.60
1	D	66	GLU	CB-CG-CD	6.21	123.16	112.60
1	C	89	HIS	CA-CB-CG	5.96	119.75	113.80
1	B	287	ASN	CA-C-O	5.92	126.45	120.88
1	D	89	HIS	CA-CB-CG	5.90	119.70	113.80
1	A	239	LEU	N-CA-CB	-5.83	100.93	110.43
1	D	181	LEU	N-CA-CB	-5.78	102.05	111.24
1	A	274	ILE	N-CA-CB	-5.72	104.16	110.51
1	B	163	LYS	CA-C-N	5.72	128.20	120.65
1	B	163	LYS	C-N-CA	5.72	128.20	120.65
1	B	287	ASN	CB-CA-C	5.69	116.80	109.80
1	C	120	PRO	CA-C-N	5.64	129.29	120.82
1	C	120	PRO	C-N-CA	5.64	129.29	120.82
1	B	120	PRO	CA-C-N	5.50	127.96	120.54
1	B	120	PRO	C-N-CA	5.50	127.96	120.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	THR	CA-CB-OG1	-5.45	101.42	109.60
1	D	337	THR	CA-CB-OG1	-5.37	101.54	109.60
1	C	163	LYS	CA-C-N	5.35	127.91	120.63
1	C	163	LYS	C-N-CA	5.35	127.91	120.63
1	B	130	THR	CA-C-O	-5.34	114.76	120.42
1	B	89	HIS	CA-CB-CG	5.32	119.11	113.80
1	C	239	LEU	N-CA-CB	-5.26	101.85	110.42
1	C	116	GLY	CA-C-O	-5.25	115.66	120.97
1	D	239	LEU	N-CA-CB	-5.24	101.88	110.42
1	B	239	LEU	N-CA-CB	-5.22	101.90	110.42
1	D	2	GLN	CB-CG-CD	-5.22	103.72	112.60
1	C	170	ASP	CA-C-N	5.22	128.24	120.31
1	C	170	ASP	C-N-CA	5.22	128.24	120.31
1	A	140	ALA	CA-C-O	-5.18	114.49	120.24
1	B	129	GLN	N-CA-C	-5.18	105.55	111.14
1	C	57	LEU	CA-C-O	-5.16	115.89	121.87
1	B	162	THR	CA-CB-OG1	-5.14	101.88	109.60
1	C	117	SER	N-CA-C	5.13	116.09	108.60
1	D	291	GLN	OE1-CD-NE2	5.13	127.73	122.60
1	D	291	GLN	CA-CB-CG	-5.12	103.87	114.10
1	B	129	GLN	CA-C-O	-5.11	115.44	120.70
1	B	40	GLU	CB-CG-CD	5.11	121.28	112.60
1	D	273	SER	CA-C-N	5.08	127.15	120.60
1	D	273	SER	C-N-CA	5.08	127.15	120.60
1	C	162	THR	CA-CB-OG1	-5.07	101.99	109.60
1	A	76	GLN	CA-C-O	-5.01	115.24	120.55
1	A	32	GLN	CB-CG-CD	5.00	121.11	112.60
1	C	129	GLN	CA-C-O	-5.00	115.57	120.82

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	2531	0	2519	26	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2510	0	2495	29	0
1	C	2456	0	2449	40	0
1	D	2508	0	2502	17	0
2	A	9	0	3	0	0
2	B	6	0	2	0	0
2	C	6	0	2	0	0
2	D	9	0	3	0	0
3	A	373	0	0	11	0
3	B	360	0	0	9	0
3	C	307	0	0	8	0
3	D	328	0	0	9	0
All	All	11403	0	9975	104	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 5.

All (104) 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:B:14:THR:HA	1:B:17:MET:HE2	1.17	1.17
1:A:274:ILE:HG13	3:A:666:HOH:O	1.48	1.11
1:C:38:MET:HE2	1:C:129:GLN:HE21	1.08	1.08
1:C:38:MET:CE	1:C:129:GLN:HE21	1.68	1.07
1:C:249:GLN:HG3	3:C:503:HOH:O	1.64	0.97
1:C:217[B]:ILE:HG22	1:C:240:ARG:O	1.73	0.88
1:A:188:ARG:HD2	1:C:125:ALA:O	1.72	0.87
1:C:38:MET:HE2	1:C:129:GLN:NE2	1.92	0.83
1:C:336:ASP:OD1	1:C:336:ASP:C	2.22	0.81
1:C:19:ARG:NH2	1:C:24:TYR:HE2	1.80	0.80
1:C:164:ALA:HA	1:D:274:ILE:HD12	1.63	0.80
1:C:34:GLN:OE1	1:C:122:ALA:HB2	1.80	0.79
1:B:17:MET:HE3	1:B:24:TYR:HB3	1.65	0.77
1:B:14:THR:CA	1:B:17:MET:HE2	2.10	0.73
1:C:250:LYS:N	3:C:503:HOH:O	2.22	0.73
1:C:35:LEU:HD12	1:C:51:ILE:HD11	1.70	0.73
1:B:180:LEU:O	1:B:181:LEU:HD12	1.89	0.72
1:C:40[B]:GLU:OE2	1:C:129:GLN:NE2	2.22	0.72
1:D:24:TYR:N	3:D:504:HOH:O	2.24	0.70
1:A:188:ARG:CD	1:C:125:ALA:O	2.40	0.69
1:C:19:ARG:HH22	1:C:24:TYR:HE2	1.38	0.69
1:B:23:GLY:C	3:B:567:HOH:O	2.35	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:MET:CE	1:C:129:GLN:NE2	2.52	0.67
1:C:229:PHE:CE1	3:D:811:HOH:O	2.46	0.67
1:C:249:GLN:C	3:C:503:HOH:O	2.38	0.66
1:D:215:VAL:HG12	3:D:811:HOH:O	1.97	0.64
1:B:17:MET:HE3	1:B:24:TYR:CB	2.29	0.62
1:D:32[A]:GLN:NE2	3:D:508:HOH:O	2.33	0.62
1:B:165[A]:HIS:HD2	1:B:170:ASP:O	1.82	0.62
1:A:274:ILE:HA	3:A:529:HOH:O	2.00	0.61
1:A:130[B]:THR:HG23	3:A:764:HOH:O	2.01	0.61
1:B:42:HIS:HD2	3:B:805:HOH:O	1.85	0.60
1:C:19:ARG:NH2	1:C:24:TYR:CE2	2.66	0.60
1:C:123:GLU:O	1:C:126:SER:HB3	2.02	0.58
1:C:165:HIS:HD2	1:C:170:ASP:O	1.87	0.58
1:B:14:THR:HA	1:B:17:MET:CE	2.12	0.57
1:C:217[B]:ILE:CG2	1:C:241:SER:HA	2.34	0.57
1:C:17:MET:HE2	1:C:26:PRO:HG3	1.87	0.56
1:A:23:GLY:C	3:A:615:HOH:O	2.48	0.56
1:C:118:GLN:NE2	3:C:508:HOH:O	2.39	0.55
1:C:163:LYS:HE3	3:C:562:HOH:O	2.07	0.54
1:C:217[B]:ILE:HD11	1:C:248:PRO:HD3	1.89	0.54
1:C:229:PHE:CD1	3:D:811:HOH:O	2.61	0.54
1:B:45[B]:GLU:OE2	1:D:153:ASN:ND2	2.39	0.53
1:A:274:ILE:CD1	1:B:274:ILE:HG12	2.37	0.53
1:B:122:ALA:CB	3:B:574:HOH:O	2.57	0.52
1:D:181:LEU:C	1:D:181:LEU:HD23	2.35	0.52
1:B:38:MET:SD	1:B:121:LEU:HD21	2.50	0.51
1:D:32[B]:GLN:HE21	1:D:32[B]:GLN:H	1.59	0.51
1:C:217[B]:ILE:HG21	1:C:241:SER:HA	1.92	0.50
1:C:291:GLN:NE2	3:C:501:HOH:O	2.21	0.50
1:A:69:GLN:HE21	1:A:73:ASN:HD21	1.60	0.50
1:A:181:LEU:C	1:A:181:LEU:HD23	2.37	0.49
1:B:17:MET:HE1	3:B:717:HOH:O	2.11	0.49
1:A:227:ARG:HD3	3:A:786:HOH:O	2.11	0.49
1:B:23:GLY:HA2	3:B:567:HOH:O	2.12	0.49
1:D:101:LEU:HD12	1:D:114[B]:ILE:HD11	1.94	0.49
1:A:315:GLN:HG2	3:A:540:HOH:O	2.13	0.48
1:A:274:ILE:CG1	3:A:666:HOH:O	2.28	0.48
1:C:98:ALA:HB2	1:C:114[A]:ILE:HG21	1.95	0.48
1:B:34:GLN:NE2	1:B:122:ALA:HB2	2.29	0.48
1:A:130[A]:THR:HG22	3:A:764:HOH:O	2.14	0.47
1:B:2:GLN:HG3	3:B:843:HOH:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:LEU:O	1:B:42:HIS:HE1	1.98	0.46
1:A:3:LYS:N	3:A:517:HOH:O	2.49	0.45
1:B:98:ALA:HB2	1:B:114[A]:ILE:HG21	1.99	0.45
1:B:23:GLY:CA	3:B:567:HOH:O	2.65	0.45
1:B:207:ILE:HD13	1:B:207:ILE:HG21	1.61	0.45
1:D:201:PRO:HD2	3:D:703:HOH:O	2.18	0.44
1:B:42:HIS:CD2	3:B:805:HOH:O	2.66	0.44
1:D:306:LEU:C	1:D:306:LEU:HD13	2.43	0.44
1:C:19:ARG:NH2	1:C:123:GLU:OE1	2.51	0.43
1:B:2:GLN:HG2	3:B:742:HOH:O	2.18	0.43
1:C:163:LYS:CE	3:C:562:HOH:O	2.66	0.43
1:A:231:LEU:O	1:A:232:GLN:C	2.61	0.43
1:B:133:LEU:C	1:B:133:LEU:HD13	2.44	0.43
1:B:165[A]:HIS:CD2	1:B:170:ASP:O	2.67	0.43
1:A:10:TYR:HA	1:A:88:LEU:HB2	2.00	0.42
1:A:247:ALA:HB1	1:A:248:PRO:HD2	2.01	0.42
1:D:60:SER:HA	1:D:63:MET:HG2	2.02	0.42
1:C:118:GLN:NE2	3:C:520:HOH:O	2.53	0.42
1:D:7:TYR:OH	3:D:501:HOH:O	2.21	0.42
1:D:320:ASN:O	1:D:324[B]:GLN:HG3	2.19	0.42
1:C:164:ALA:O	1:D:274:ILE:HB	2.20	0.42
1:B:46:MET:HE2	1:B:133:LEU:HD22	2.02	0.42
1:C:226:VAL:HA	1:C:229:PHE:CD2	2.55	0.42
1:C:274:ILE:HG12	1:D:274:ILE:HG12	2.02	0.41
1:B:8:VAL:HB	1:B:51:ILE:HD13	2.03	0.41
1:A:71:ILE:HG21	1:A:87[A]:ILE:HD13	2.03	0.41
1:C:46:MET:HE3	1:C:46:MET:HB3	1.95	0.41
1:B:269:ASN:HB3	1:B:280:MET:HE1	2.03	0.41
1:C:306:LEU:HD13	1:C:306:LEU:C	2.45	0.41
1:A:306:LEU:C	1:A:306:LEU:HD13	2.46	0.41
1:D:274:ILE:HA	3:D:603:HOH:O	2.20	0.41
1:A:69:GLN:HE21	1:A:73:ASN:ND2	2.19	0.41
1:A:69:GLN:HA	1:A:104:MET:HE1	2.03	0.41
1:C:60:SER:HA	1:C:63:MET:HG2	2.02	0.41
1:D:80[A]:ASP:OD1	3:D:502:HOH:O	2.22	0.41
1:C:274:ILE:HD12	1:C:274:ILE:HA	1.80	0.40
1:A:275[B]:SER:OG	1:B:165[B]:HIS:CD2	2.75	0.40
1:A:113:ILE:HG12	1:A:148[B]:SER:OG	2.22	0.40
1:A:311:TYR:O	1:A:315:GLN:HG3	2.21	0.40
1:A:17:MET:CE	3:A:707:HOH:O	2.69	0.40
1:A:43:ARG:HD3	3:A:798: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	329/338 (97%)	317 (96%)	12 (4%)	0	100	100
1	B	327/338 (97%)	314 (96%)	13 (4%)	0	100	100
1	C	316/338 (94%)	307 (97%)	9 (3%)	0	100	100
1	D	324/338 (96%)	315 (97%)	9 (3%)	0	100	100
All	All	1296/1352 (96%)	1253 (97%)	43 (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	278/282 (99%)	274 (99%)	4 (1%)	59	59
1	B	276/282 (98%)	273 (99%)	3 (1%)	65	67
1	C	268/282 (95%)	267 (100%)	1 (0%)	84	87
1	D	276/282 (98%)	271 (98%)	5 (2%)	51	50
All	All	1098/1128 (97%)	1085 (99%)	13 (1%)	63	63

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	153	ASN
1	A	188	ARG
1	A	197	THR
1	A	207	ILE
1	B	124	ASP
1	B	133	LEU
1	B	280	MET
1	C	34	GLN
1	D	2	GLN
1	D	153	ASN
1	D	181	LEU
1	D	198	SER
1	D	280	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	73	ASN
1	A	78	ASN
1	A	145	ASN
1	A	154	GLN
1	A	165	HIS
1	A	232	GLN
1	A	246	ASN
1	A	328	GLN
1	B	34	GLN
1	B	42	HIS
1	B	52	HIS
1	B	73	ASN
1	B	129	GLN
1	B	145	ASN
1	B	153	ASN
1	B	259	ASN
1	C	52	HIS
1	C	118	GLN
1	C	129	GLN
1	C	145	ASN
1	C	154	GLN
1	C	199	ASN
1	C	324	GLN
1	D	18	GLN
1	D	34	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	70	HIS
1	D	145	ASN
1	D	165	HIS
1	D	199	ASN
1	D	232	GLN
1	D	249	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](#)

10 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	FMT	C	402	-	2,2,2	0.18	0	1,1,1	0.23	0
2	FMT	C	401	-	2,2,2	0.42	0	1,1,1	0.01	0
2	FMT	D	401	-	2,2,2	0.93	0	1,1,1	0.46	0
2	FMT	D	402	-	2,2,2	0.29	0	1,1,1	0.14	0
2	FMT	A	402	-	2,2,2	0.92	0	1,1,1	0.18	0
2	FMT	A	401	-	2,2,2	0.55	0	1,1,1	0.03	0
2	FMT	B	402	-	2,2,2	0.31	0	1,1,1	0.19	0
2	FMT	D	403	-	2,2,2	0.63	0	1,1,1	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FMT	A	403	-	2,2,2	0.37	0	1,1,1	0.05	0
2	FMT	B	401	-	2,2,2	0.41	0	1,1,1	0.21	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	329/338 (97%)	-0.08	12 (3%)	46	49	10, 23, 44, 96	4 (1%)
1	B	322/338 (95%)	-0.07	19 (5%)	28	30	9, 20, 51, 100	9 (2%)
1	C	317/338 (93%)	-0.06	10 (3%)	50	54	10, 23, 49, 100	5 (1%)
1	D	323/338 (95%)	-0.19	5 (1%)	72	75	9, 21, 40, 75	7 (2%)
All	All	1291/1352 (95%)	-0.10	46 (3%)	46	49	9, 22, 47, 100	25 (1%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	187	ILE	4.8
1	B	125	ALA	4.5
1	B	283	TYR	4.5
1	B	126	SER	4.4
1	B	184	GLY	4.1
1	B	285	THR	3.9
1	B	284	ALA	3.9
1	B	183	ALA	3.5
1	C	125	ALA	3.4
1	D	20	SER	3.4
1	D	198	SER	3.2
1	B	23	GLY	3.1
1	B	181	LEU	3.1
1	A	199	ASN	3.1
1	C	184	GLY	3.0
1	C	25	ILE	3.0
1	A	198	SER	2.9
1	C	19	ARG	2.9
1	B	281	GLY	2.8
1	B	169	PHE	2.8
1	B	122	ALA	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	187	ILE	2.7
1	B	199	ASN	2.6
1	C	181	LEU	2.6
1	C	45	GLU	2.6
1	A	197	THR	2.6
1	A	195	SER	2.6
1	C	336	ASP	2.5
1	A	285	THR	2.5
1	D	337	THR	2.5
1	C	24	TYR	2.5
1	A	169	PHE	2.5
1	B	282	GLY	2.4
1	A	52	HIS	2.4
1	B	118	GLN	2.4
1	A	55	ALA	2.3
1	D	169	PHE	2.3
1	A	201	PRO	2.3
1	A	22	ASN	2.3
1	C	15	ILE	2.2
1	B	22	ASN	2.2
1	A	81	LEU	2.2
1	B	287	ASN	2.1
1	B	2	GLN	2.0
1	C	183	ALA	2.0
1	B	337	THR	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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	FMT	C	401	3/3	0.96	0.08	27,27,29,35	0
2	FMT	A	402	3/3	0.97	0.05	19,19,19,20	0
2	FMT	B	401	3/3	0.97	0.07	20,20,22,23	0
2	FMT	A	401	3/3	0.97	0.06	17,17,22,22	0
2	FMT	C	402	3/3	0.97	0.06	28,28,29,37	0
2	FMT	D	403	3/3	0.97	0.07	26,26,30,32	0
2	FMT	D	402	3/3	0.98	0.06	20,20,23,23	0
2	FMT	D	401	3/3	0.99	0.03	19,19,19,20	0
2	FMT	A	403	3/3	0.99	0.05	22,22,23,28	0
2	FMT	B	402	3/3	0.99	0.05	18,18,22,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.