



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:21 am BST

PDB ID : 6NXD
Title : TYPE I L-ASPARAGINASE FROM ESCHERICHIA COLI IN COMPLEX WITH CITRATE AT PH 4
Authors : Lubkowski, J.; Wlodawer, A.
Deposited on : 2019-02-08
Resolution : 1.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

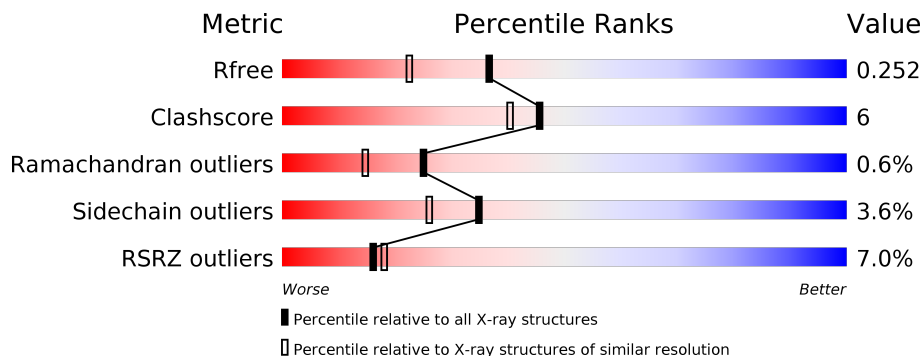
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 on 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	358	 5% 74% 11% • 15%
1	B	358	 7% 79% 11% • 9%
1	C	358	 8% 73% 13% • 13%
1	D	358	 4% 77% 13% • 9%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10411 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 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	305	2336	1482	398	446	10	0	0	0
1	B	325	2491	1579	428	472	12	0	0	0
1	C	311	2394	1522	406	454	12	0	1	0
1	D	324	2480	1574	423	472	11	0	1	0

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP P0A962
A	-18	GLY	-	expression tag	UNP P0A962
A	-17	SER	-	expression tag	UNP P0A962
A	-16	SER	-	expression tag	UNP P0A962
A	-15	HIS	-	expression tag	UNP P0A962
A	-14	HIS	-	expression tag	UNP P0A962
A	-13	HIS	-	expression tag	UNP P0A962
A	-12	HIS	-	expression tag	UNP P0A962
A	-11	HIS	-	expression tag	UNP P0A962
A	-10	HIS	-	expression tag	UNP P0A962
A	-9	SER	-	expression tag	UNP P0A962
A	-8	SER	-	expression tag	UNP P0A962
A	-7	GLY	-	expression tag	UNP P0A962
A	-6	LEU	-	expression tag	UNP P0A962
A	-5	VAL	-	expression tag	UNP P0A962
A	-4	PRO	-	expression tag	UNP P0A962
A	-3	ARG	-	expression tag	UNP P0A962
A	-2	GLY	-	expression tag	UNP P0A962
A	-1	SER	-	expression tag	UNP P0A962
A	0	HIS	-	expression tag	UNP P0A962
B	-19	MET	-	initiating methionine	UNP P0A962

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP P0A962
B	-17	SER	-	expression tag	UNP P0A962
B	-16	SER	-	expression tag	UNP P0A962
B	-15	HIS	-	expression tag	UNP P0A962
B	-14	HIS	-	expression tag	UNP P0A962
B	-13	HIS	-	expression tag	UNP P0A962
B	-12	HIS	-	expression tag	UNP P0A962
B	-11	HIS	-	expression tag	UNP P0A962
B	-10	HIS	-	expression tag	UNP P0A962
B	-9	SER	-	expression tag	UNP P0A962
B	-8	SER	-	expression tag	UNP P0A962
B	-7	GLY	-	expression tag	UNP P0A962
B	-6	LEU	-	expression tag	UNP P0A962
B	-5	VAL	-	expression tag	UNP P0A962
B	-4	PRO	-	expression tag	UNP P0A962
B	-3	ARG	-	expression tag	UNP P0A962
B	-2	GLY	-	expression tag	UNP P0A962
B	-1	SER	-	expression tag	UNP P0A962
B	0	HIS	-	expression tag	UNP P0A962
C	-19	MET	-	initiating methionine	UNP P0A962
C	-18	GLY	-	expression tag	UNP P0A962
C	-17	SER	-	expression tag	UNP P0A962
C	-16	SER	-	expression tag	UNP P0A962
C	-15	HIS	-	expression tag	UNP P0A962
C	-14	HIS	-	expression tag	UNP P0A962
C	-13	HIS	-	expression tag	UNP P0A962
C	-12	HIS	-	expression tag	UNP P0A962
C	-11	HIS	-	expression tag	UNP P0A962
C	-10	HIS	-	expression tag	UNP P0A962
C	-9	SER	-	expression tag	UNP P0A962
C	-8	SER	-	expression tag	UNP P0A962
C	-7	GLY	-	expression tag	UNP P0A962
C	-6	LEU	-	expression tag	UNP P0A962
C	-5	VAL	-	expression tag	UNP P0A962
C	-4	PRO	-	expression tag	UNP P0A962
C	-3	ARG	-	expression tag	UNP P0A962
C	-2	GLY	-	expression tag	UNP P0A962
C	-1	SER	-	expression tag	UNP P0A962
C	0	HIS	-	expression tag	UNP P0A962
D	-19	MET	-	initiating methionine	UNP P0A962
D	-18	GLY	-	expression tag	UNP P0A962
D	-17	SER	-	expression tag	UNP P0A962

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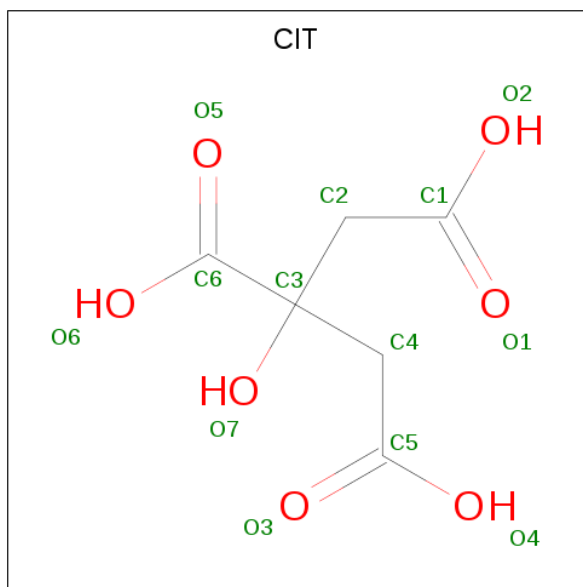
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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP P0A962
D	-15	HIS	-	expression tag	UNP P0A962
D	-14	HIS	-	expression tag	UNP P0A962
D	-13	HIS	-	expression tag	UNP P0A962
D	-12	HIS	-	expression tag	UNP P0A962
D	-11	HIS	-	expression tag	UNP P0A962
D	-10	HIS	-	expression tag	UNP P0A962
D	-9	SER	-	expression tag	UNP P0A962
D	-8	SER	-	expression tag	UNP P0A962
D	-7	GLY	-	expression tag	UNP P0A962
D	-6	LEU	-	expression tag	UNP P0A962
D	-5	VAL	-	expression tag	UNP P0A962
D	-4	PRO	-	expression tag	UNP P0A962
D	-3	ARG	-	expression tag	UNP P0A962
D	-2	GLY	-	expression tag	UNP P0A962
D	-1	SER	-	expression tag	UNP P0A962
D	0	HIS	-	expression tag	UNP P0A962

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

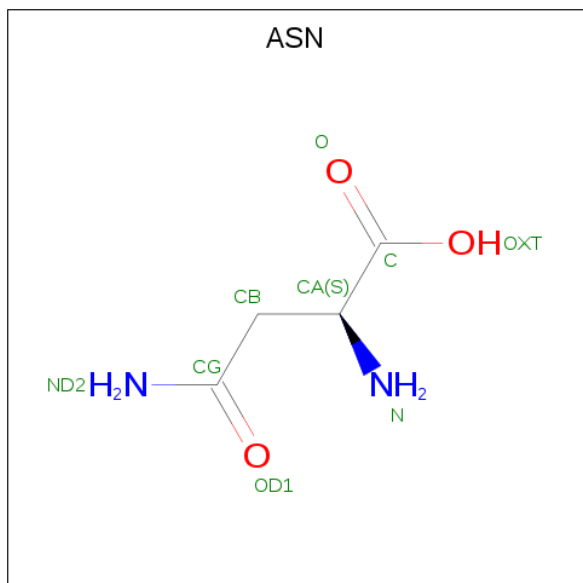
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	4	Total Cl 4 4	0	0
2	A	4	Total Cl 4 4	0	0
2	D	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



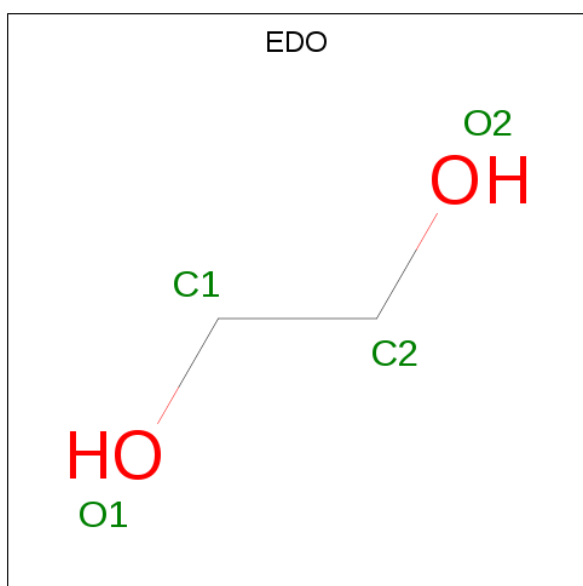
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	C	1	Total	C	O	0	0
			12	6	6		
3	D	1	Total	C	O	0	0
			12	6	6		

- Molecule 4 is ASPARAGINE (three-letter code: ASN) (formula: $C_4H_8N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			9	4	2	3		
4	B	1	Total	C	N	O	0	0
			9	4	2	3		
4	C	1	Total	C	N	O	0	0
			9	4	2	3		
4	D	1	Total	C	N	O	0	0
			9	4	2	3		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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

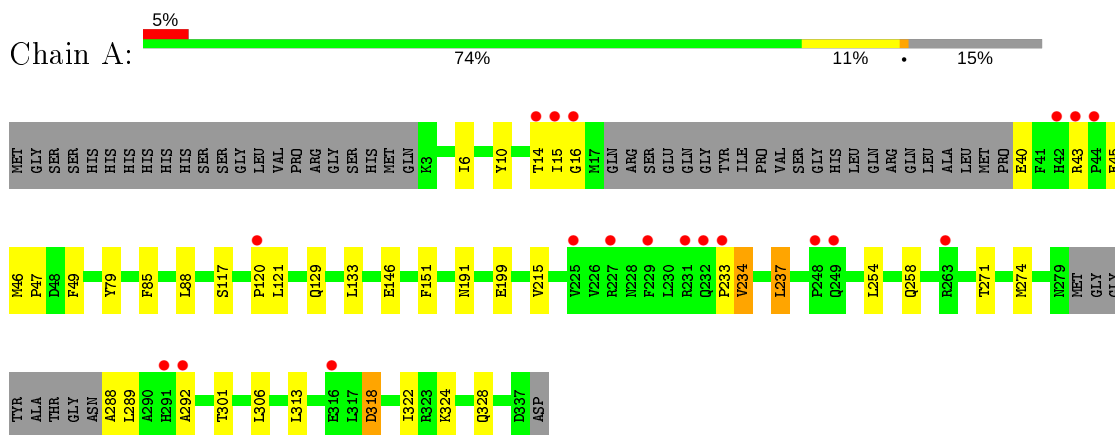
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	129	Total O 129 129	0	0
6	B	150	Total O 150 150	0	0
6	C	124	Total O 124 124	0	0
6	D	161	Total O 161 161	0	0

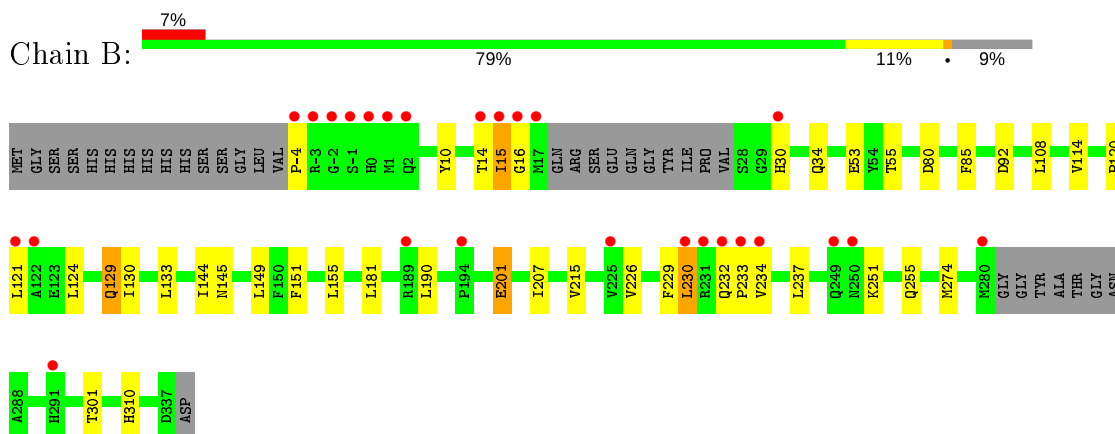
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

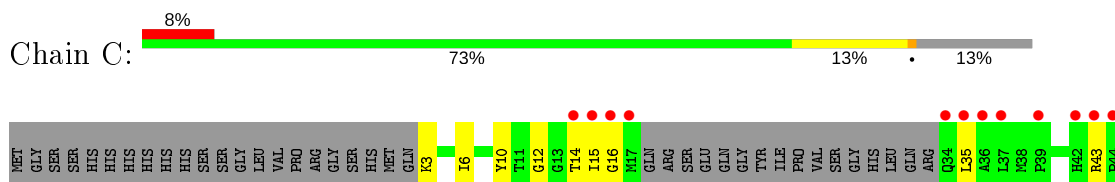
- Molecule 1: L-asparaginase 1

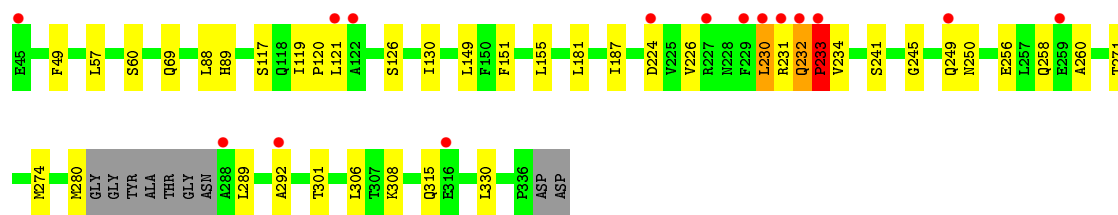


- Molecule 1: L-asparaginase 1

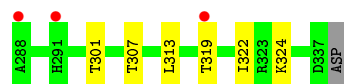
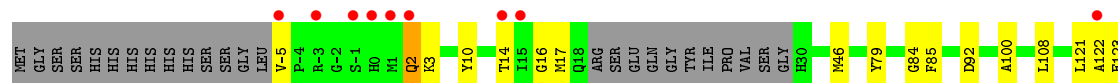
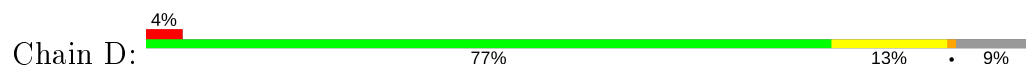


- Molecule 1: L-asparaginase 1





- Molecule 1: L-asparaginase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.31Å 89.76Å 93.08Å 90.00° 117.03° 90.00°	Depositor
Resolution (Å)	45.17 – 1.90 45.13 – 1.90	Depositor EDS
% Data completeness (in resolution range)	90.7 (45.17-1.90) 90.7 (45.13-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.46 (at 1.89Å)	Xtrriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.203 , 0.244 0.213 , 0.252	Depositor DCC
R_{free} test set	4749 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	18.3	Xtrriage
Anisotropy	0.121	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 55.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.148 for l,-k,h	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10411	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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: CL, EDO, CIT

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	0.77	0/2387	0.89	1/3251 (0.0%)
1	B	0.75	0/2546	0.89	0/3465
1	C	0.75	0/2447	0.89	2/3332 (0.1%)
1	D	0.76	0/2537	0.92	1/3457 (0.0%)
All	All	0.76	0/9917	0.90	4/13505 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	233	PRO	N-CA-CB	-5.71	96.32	102.60
1	A	271	THR	CA-CB-OG1	-5.59	97.26	109.00
1	C	271	THR	CA-CB-OG1	-5.42	97.63	109.00
1	D	125	ARG	NE-CZ-NH2	-5.14	117.73	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2336	0	2286	27	0
1	B	2491	0	2453	30	0
1	C	2394	0	2369	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2480	0	2435	40	0
2	A	4	0	0	1	0
2	B	4	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	12	0	5	1	0
3	B	12	0	5	1	0
3	C	12	0	5	0	0
3	D	12	0	5	3	0
4	A	9	0	5	0	0
4	B	9	0	5	0	0
4	C	9	0	5	0	0
4	D	9	0	5	0	0
5	A	12	0	18	3	0
5	B	12	0	18	1	0
5	C	8	0	12	1	0
5	D	20	0	30	1	0
6	A	129	0	0	2	0
6	B	150	0	0	4	0
6	C	124	0	0	1	0
6	D	161	0	0	1	0
All	All	10411	0	9661	125	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 (125) 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:10:TYR:OH	1:B:16:GLY:HA3	1.80	0.82
1:D:14:THR:HA	1:D:17:MET:HE3	1.60	0.81
1:C:232:GLN:H	1:C:233:PRO:HD3	1.50	0.76
1:B:274:MET:HE3	1:D:274:MET:HB2	1.71	0.70
1:D:-5:VAL:HA	1:D:144:ILE:HG12	1.73	0.69
1:A:318:ASP:OD1	6:A:1101:HOH:O	2.11	0.69
1:D:14:THR:HA	1:D:17:MET:CE	2.24	0.67
1:B:229:PHE:HB3	1:B:234:VAL:HG21	1.77	0.66
1:B:215:VAL:CG2	1:B:237:LEU:HD21	2.26	0.66
1:C:181:LEU:HD21	1:C:187:ILE:HG23	1.77	0.65
1:B:207:ILE:HG23	1:B:310:HIS:HB3	1.80	0.63
1:B:274:MET:CE	1:D:274:MET:HB2	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:GLU:CD	6:B:1101:HOH:O	2.36	0.63
1:C:10:TYR:OH	1:C:16:GLY:HA3	2.00	0.62
1:D:234:VAL:HG11	1:D:237:LEU:HD13	1.80	0.62
1:D:227:ARG:N	1:D:256:GLU:OE2	2.33	0.61
1:A:40:GLU:O	1:A:43:ARG:HG2	2.01	0.61
1:D:319:THR:HG22	6:D:1244:HOH:O	2.01	0.60
1:B:92:ASP:OD2	3:B:1005:CIT:H21	2.01	0.59
1:D:-5:VAL:CB	1:D:144:ILE:HD11	2.32	0.59
1:C:241[A]:SER:OG	1:C:245:GLY:HA2	2.04	0.58
1:B:215:VAL:HG21	1:B:237:LEU:HD21	1.85	0.58
1:B:129:GLN:HB2	6:B:1156:HOH:O	2.04	0.57
1:D:10:TYR:OH	1:D:16:GLY:HA3	2.04	0.56
1:B:-4:PRO:HD2	1:B:144:ILE:HG12	1.88	0.56
1:A:10:TYR:OH	1:A:16:GLY:HA3	2.04	0.56
1:D:215[A]:VAL:HG12	1:D:239:LEU:HD23	1.87	0.56
1:A:301:THR:HA	5:A:1008:EDO:H12	1.88	0.55
1:D:164:ALA:HB2	1:D:274:MET:HE1	1.88	0.55
1:A:15:ILE:HD13	1:A:88:LEU:HD22	1.88	0.55
1:A:215:VAL:HG23	1:A:237:LEU:CD1	2.37	0.55
1:C:232:GLN:H	1:C:233:PRO:CD	2.19	0.55
1:C:230:LEU:HD21	1:C:260:ALA:HB2	1.89	0.55
1:A:199:GLU:OE2	6:A:1102:HOH:O	2.19	0.54
1:A:15:ILE:O	1:A:121:LEU:CB	2.56	0.53
1:C:15:ILE:HD13	1:C:88:LEU:HD22	1.91	0.53
1:B:215:VAL:HG23	1:B:237:LEU:HD21	1.92	0.52
1:D:230:LEU:HD11	1:D:260:ALA:HA	1.92	0.52
1:A:121:LEU:CB	1:A:129:GLN:HE22	2.23	0.52
1:C:14:THR:HG23	1:C:120:PRO:HD3	1.92	0.52
1:B:226:VAL:O	1:B:230:LEU:HD23	2.09	0.51
1:D:215[A]:VAL:HG11	1:D:239:LEU:HD22	1.93	0.51
1:B:233:PRO:O	1:B:234:VAL:HG23	2.10	0.51
1:C:230:LEU:HD21	1:C:260:ALA:CB	2.41	0.51
1:A:45:GLU:HB2	1:B:124:LEU:HD22	1.93	0.50
1:A:215:VAL:CG2	1:A:237:LEU:HD11	2.41	0.50
1:A:14:THR:HG22	1:A:120:PRO:N	2.26	0.50
1:C:15:ILE:HA	1:C:117:SER:OG	2.12	0.50
1:A:234:VAL:HG11	1:A:237:LEU:HD23	1.92	0.50
1:C:258:GLN:NE2	1:C:292:ALA:HA	2.27	0.49
1:C:15:ILE:O	1:C:121:LEU:HB2	2.12	0.49
1:C:6:ILE:O	1:C:49:PHE:HA	2.12	0.49
1:B:121:LEU:HD11	1:B:129:GLN:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:ASN:HB2	1:D:197:HIS:HE1	1.76	0.49
1:B:80:ASP:OD1	6:B:1101:HOH:O	2.20	0.49
1:C:232:GLN:N	1:C:233:PRO:CD	2.76	0.49
1:C:60:SER:HB2	1:C:89:HIS:CE1	2.47	0.49
1:C:230:LEU:HD11	1:C:260:ALA:HA	1.95	0.48
1:B:14:THR:HG23	1:B:120:PRO:HD3	1.95	0.48
1:C:301:THR:HA	5:C:1004:EDO:H12	1.95	0.48
1:B:155:LEU:HB3	1:B:181:LEU:HB3	1.95	0.48
1:D:215[A]:VAL:CG1	1:D:239:LEU:CD2	2.91	0.48
1:C:280:MET:CE	1:C:289:LEU:HB2	2.44	0.48
1:D:215[A]:VAL:CG1	1:D:239:LEU:HD22	2.43	0.48
1:A:15:ILE:HA	1:A:117:SER:OG	2.13	0.47
1:A:14:THR:CG2	1:A:120:PRO:HD3	2.44	0.47
1:C:14:THR:CG2	1:C:120:PRO:HD3	2.45	0.47
1:A:215:VAL:CG2	1:A:237:LEU:CD1	2.92	0.47
1:D:2:GLN:HE21	1:D:2:GLN:HB2	1.54	0.47
1:C:15:ILE:CA	1:C:117:SER:OG	2.63	0.47
1:D:46:MET:CE	1:D:133:LEU:HD22	2.44	0.47
1:A:79:TYR:HA	1:A:85:PHE:CZ	2.50	0.46
1:A:191:ASN:HD22	1:D:193:PRO:HD3	1.80	0.46
1:A:258:GLN:OE1	1:A:292:ALA:HA	2.16	0.46
1:D:121:LEU:HD11	1:D:129:GLN:HG3	1.98	0.45
1:D:233:PRO:O	1:D:234:VAL:HG23	2.17	0.45
1:D:85:PHE:N	1:D:85:PHE:CD1	2.85	0.45
1:A:274:MET:HE1	6:C:1198:HOH:O	2.17	0.45
1:D:108:LEU:O	1:D:145:ASN:HB3	2.17	0.44
1:D:164:ALA:HB2	1:D:274:MET:CE	2.47	0.44
1:C:43:ARG:NH2	1:D:122:ALA:O	2.51	0.44
1:D:145:ASN:HB2	1:D:197:HIS:CE1	2.52	0.44
1:D:234:VAL:HG11	1:D:237:LEU:CD1	2.44	0.44
2:A:1003:CL:CL	5:A:1007:EDO:O1	2.73	0.43
1:A:324:LYS:O	1:A:328:GLN:HG3	2.18	0.43
1:D:100:ALA:HA	1:D:307:THR:HB	2.00	0.43
1:B:30:HIS:O	1:B:34:GLN:HG2	2.17	0.43
1:C:226:VAL:CG1	1:C:256:GLU:HB3	2.48	0.43
1:C:250:ASN:OD1	1:C:250:ASN:C	2.56	0.43
1:D:301:THR:HA	5:D:1004:EDO:H21	2.00	0.43
1:A:146:GLU:HG2	5:A:1007:EDO:H22	2.00	0.43
1:D:217:ILE:HG22	1:D:242:TYR:CZ	2.54	0.43
1:D:92:ASP:OD2	3:D:1002:CIT:H21	2.19	0.43
1:A:313:LEU:HD23	1:A:322:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:THR:O	1:B:120:PRO:HA	2.18	0.43
1:D:155:LEU:HB3	1:D:181:LEU:HB3	2.01	0.43
1:D:279:ASN:HD22	1:D:279:ASN:C	2.22	0.42
1:D:215[A]:VAL:HG12	1:D:239:LEU:CD2	2.50	0.42
1:A:6:ILE:O	1:A:49:PHE:HA	2.19	0.42
1:B:14:THR:CG2	1:B:120:PRO:HD3	2.48	0.42
1:C:308:LYS:HE3	1:C:330:LEU:HD12	2.01	0.42
1:D:249:GLN:CA	1:D:249:GLN:HE21	2.32	0.42
1:B:85:PHE:CD1	1:B:85:PHE:N	2.88	0.42
1:C:12:GLY:HA2	1:C:57:LEU:HD22	2.00	0.42
1:A:46:MET:HE3	1:A:47:PRO:HD2	2.02	0.42
1:B:121:LEU:CD1	1:B:129:GLN:HG3	2.51	0.41
1:B:15:ILE:HG13	6:B:1170:HOH:O	2.19	0.41
1:D:313:LEU:HD23	1:D:322:ILE:HD13	2.02	0.41
1:D:84:GLY:C	1:D:85:PHE:CD1	2.94	0.41
1:B:114:VAL:O	1:B:149:LEU:HA	2.21	0.41
1:B:108:LEU:O	1:B:145:ASN:HB3	2.21	0.41
1:B:130:ILE:HD12	1:B:130:ILE:HA	1.91	0.41
1:B:10:TYR:HB3	1:B:53:GLU:HA	2.02	0.41
1:C:119:ILE:HB	1:C:126:SER:HA	2.02	0.41
1:B:301:THR:HA	5:B:1007:EDO:H21	2.03	0.41
1:C:14:THR:HG22	1:C:120:PRO:N	2.36	0.41
1:C:149:LEU:C	1:C:149:LEU:HD23	2.41	0.41
1:A:254:LEU:HD21	1:A:288:ALA:HB1	2.03	0.41
1:D:17:MET:HE1	3:D:1002:CIT:O7	2.21	0.41
1:C:130:ILE:HA	1:C:130:ILE:HD12	1.92	0.40
3:D:1002:CIT:O2	3:D:1002:CIT:C6	2.69	0.40
3:A:1005:CIT:C6	3:A:1005:CIT:O2	2.69	0.40
1:C:155:LEU:HB3	1:C:181:LEU:HB3	2.03	0.40
1:A:14:THR:CG2	1:A:120:PRO:CD	3.00	0.40
1:D:79:TYR:HA	1:D:85:PHE:CZ	2.56	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	299/358 (84%)	287 (96%)	11 (4%)	1 (0%)	41	31
1	B	319/358 (89%)	308 (97%)	10 (3%)	1 (0%)	41	31
1	C	306/358 (86%)	294 (96%)	9 (3%)	3 (1%)	15	6
1	D	319/358 (89%)	309 (97%)	8 (2%)	2 (1%)	25	15
All	All	1243/1432 (87%)	1198 (96%)	38 (3%)	7 (1%)	25	15

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	231	ARG
1	D	232	GLN
1	B	232	GLN
1	A	233	PRO
1	C	233	PRO
1	D	233	PRO
1	C	232	GLN

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	250/298 (84%)	243 (97%)	7 (3%)	43	36
1	B	267/298 (90%)	257 (96%)	10 (4%)	34	25
1	C	258/298 (87%)	246 (95%)	12 (5%)	26	16
1	D	265/298 (89%)	256 (97%)	9 (3%)	37	28
All	All	1040/1192 (87%)	1002 (96%)	38 (4%)	35	25

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	LEU

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Mol	Chain	Res	Type
1	A	151	PHE
1	A	234	VAL
1	A	237	LEU
1	A	289	LEU
1	A	306	LEU
1	A	318	ASP
1	B	15	ILE
1	B	55	THR
1	B	129	GLN
1	B	133	LEU
1	B	151	PHE
1	B	190	LEU
1	B	201	GLU
1	B	230	LEU
1	B	251	LYS
1	B	255	GLN
1	C	3	LYS
1	C	35	LEU
1	C	69	GLN
1	C	151	PHE
1	C	224	ASP
1	C	230	LEU
1	C	233	PRO
1	C	234	VAL
1	C	249	GLN
1	C	274	MET
1	C	306	LEU
1	C	315	GLN
1	D	2	GLN
1	D	3	LYS
1	D	123	GLU
1	D	151	PHE
1	D	202	LEU
1	D	230	LEU
1	D	249	GLN
1	D	279	ASN
1	D	324	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	GLN

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Mol	Chain	Res	Type
1	B	152	ASN
1	B	153	ASN
1	B	249	GLN
1	B	258	GLN
1	B	328	GLN
1	C	70	HIS
1	C	186	HIS
1	C	258	GLN
1	C	315	GLN
1	D	2	GLN
1	D	249	GLN
1	D	250	ASN
1	D	255	GLN
1	D	279	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 10 are monoatomic - leaving 21 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
5	EDO	C	1005	-	3,3,3	0.36	0	2,2,2	0.43	0
3	CIT	C	1002	1	4,11,12	0.79	0	4,15,17	1.09	0
5	EDO	D	1005	-	3,3,3	0.56	0	2,2,2	0.83	0
3	CIT	A	1005	1	4,11,12	0.73	0	4,15,17	1.02	0
5	EDO	D	1004	-	3,3,3	0.46	0	2,2,2	0.62	0
3	CIT	B	1005	1	5,11,12	1.23	1 (20%)	4,15,17	1.44	1 (25%)
5	EDO	B	1009	-	3,3,3	0.33	0	2,2,2	0.45	0
5	EDO	D	1008	-	3,3,3	0.55	0	2,2,2	0.29	0
5	EDO	B	1007	-	3,3,3	0.33	0	2,2,2	0.46	0
5	EDO	A	1007	-	3,3,3	0.10	0	2,2,2	0.14	0
5	EDO	D	1007	-	3,3,3	0.45	0	2,2,2	0.40	0
5	EDO	A	1008	-	3,3,3	0.20	0	2,2,2	0.37	0
5	EDO	B	1008	-	3,3,3	0.24	0	2,2,2	0.46	0
5	EDO	C	1004	-	3,3,3	0.29	0	2,2,2	0.38	0
5	EDO	A	1009	-	3,3,3	0.36	0	2,2,2	0.47	0
5	EDO	D	1006	-	3,3,3	0.57	0	2,2,2	0.52	0
3	CIT	D	1002	1	4,11,12	0.98	0	4,15,17	1.23	1 (25%)

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
5	EDO	C	1005	-	-	0/1/1/1	-
3	CIT	C	1002	1	-	1/7/15/16	-
5	EDO	D	1005	-	-	1/1/1/1	-
3	CIT	A	1005	1	-	1/7/15/16	-
5	EDO	D	1004	-	-	0/1/1/1	-
3	CIT	B	1005	1	-	0/7/15/16	-
5	EDO	B	1009	-	-	0/1/1/1	-
5	EDO	D	1008	-	-	0/1/1/1	-
5	EDO	B	1007	-	-	0/1/1/1	-
5	EDO	A	1007	-	-	1/1/1/1	-
5	EDO	D	1007	-	-	1/1/1/1	-
5	EDO	A	1008	-	-	0/1/1/1	-
5	EDO	B	1008	-	-	1/1/1/1	-
5	EDO	C	1004	-	-	0/1/1/1	-
5	EDO	A	1009	-	-	0/1/1/1	-
5	EDO	D	1006	-	-	0/1/1/1	-
3	CIT	D	1002	1	-	1/7/15/16	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1005	CIT	O4-C5	-2.46	1.29	1.42

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1005	CIT	O4-C5-C4	2.41	117.82	111.39
3	D	1002	CIT	O3-C5-C4	-2.16	120.34	126.78

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	1008	EDO	O1-C1-C2-O2
5	D	1007	EDO	O1-C1-C2-O2
3	D	1002	CIT	C3-C4-C5-O3
3	C	1002	CIT	C3-C4-C5-O3
3	A	1005	CIT	C3-C4-C5-O3
5	A	1007	EDO	O1-C1-C2-O2
5	D	1005	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1005	CIT	1	0
5	D	1004	EDO	1	0
3	B	1005	CIT	1	0
5	B	1007	EDO	1	0
5	A	1007	EDO	2	0
5	A	1008	EDO	1	0
5	C	1004	EDO	1	0
3	D	1002	CIT	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	305/358 (85%)	0.29	19 (6%) 20 23	10, 19, 46, 84	0
1	B	325/358 (90%)	0.30	26 (8%) 12 13	10, 18, 46, 74	0
1	C	311/358 (86%)	0.39	27 (8%) 10 11	10, 20, 53, 79	0
1	D	324/358 (90%)	0.23	16 (4%) 29 33	10, 18, 44, 74	0
All	All	1265/1432 (88%)	0.30	88 (6%) 16 18	10, 19, 48, 84	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	233	PRO	11.0
1	C	39	PRO	8.2
1	D	233	PRO	6.4
1	B	15	ILE	6.0
1	D	122	ALA	5.8
1	C	37	LEU	5.2
1	C	231	ARG	5.1
1	B	232	GLN	4.7
1	C	232	GLN	4.7
1	B	231	ARG	4.4
1	D	0	HIS	4.4
1	A	14	THR	4.4
1	C	42	HIS	4.2
1	B	122	ALA	3.8
1	B	1	MET	3.8
1	A	16	GLY	3.8
1	D	-1	SER	3.6
1	B	291	HIS	3.6
1	B	14	THR	3.5
1	C	316	GLU	3.5
1	C	16	GLY	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	231	ARG	3.5
1	A	42	HIS	3.4
1	A	227	ARG	3.4
1	D	1	MET	3.4
1	D	232	GLN	3.4
1	C	14	THR	3.4
1	D	288	ALA	3.3
1	C	44	PRO	3.3
1	A	249	GLN	3.2
1	B	234	VAL	3.2
1	D	14	THR	3.2
1	A	229	PHE	3.2
1	B	121	LEU	3.1
1	A	233	PRO	3.1
1	D	-5	VAL	3.1
1	C	35	LEU	3.1
1	C	230	LEU	3.1
1	A	292	ALA	3.1
1	B	194	PRO	3.1
1	B	0	HIS	3.1
1	C	229	PHE	3.0
1	D	2	GLN	2.9
1	B	2	GLN	2.9
1	C	292	ALA	2.9
1	A	43	ARG	2.9
1	B	249	GLN	2.8
1	D	-3	ARG	2.8
1	C	43	ARG	2.8
1	A	44	PRO	2.7
1	C	233	PRO	2.7
1	B	230	LEU	2.7
1	A	316	GLU	2.7
1	D	15	ILE	2.7
1	D	249	GLN	2.7
1	B	16	GLY	2.6
1	B	225	VAL	2.6
1	C	15	ILE	2.5
1	B	17	MET	2.5
1	C	227	ARG	2.5
1	B	-2	GLY	2.5
1	C	259	GLU	2.5
1	A	291	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	194	PRO	2.4
1	C	288	ALA	2.4
1	C	121	LEU	2.4
1	A	232	GLN	2.4
1	C	122	ALA	2.3
1	B	-1	SER	2.2
1	C	17	MET	2.2
1	A	225	VAL	2.2
1	A	15	ILE	2.2
1	B	280	MET	2.2
1	B	-3	ARG	2.2
1	D	291	HIS	2.2
1	B	30	HIS	2.2
1	C	36	ALA	2.2
1	A	248	PRO	2.1
1	B	189	ARG	2.1
1	C	249	GLN	2.1
1	C	224	ASP	2.1
1	C	34	GLN	2.1
1	B	250	ASN	2.1
1	B	-4	PRO	2.1
1	D	319	THR	2.0
1	A	263	ARG	2.0
1	A	120	PRO	2.0
1	C	45	GLU	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 carbohydrates 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(\AA^2)	Q<0.9
5	EDO	D	1006	4/4	0.72	0.17	31,33,35,37	0
5	EDO	D	1007	4/4	0.81	0.10	31,37,37,37	0
3	CIT	B	1005	12/13	0.87	0.16	22,27,32,35	0
5	EDO	D	1005	4/4	0.90	0.13	18,20,20,22	0
5	EDO	A	1007	4/4	0.90	0.16	37,37,37,40	0
3	CIT	D	1002	12/13	0.91	0.13	18,22,27,30	0
5	EDO	D	1008	4/4	0.91	0.12	15,15,16,17	0
3	CIT	C	1002	12/13	0.91	0.13	17,22,28,33	0
3	CIT	A	1005	12/13	0.92	0.10	19,23,28,31	0
5	EDO	B	1008	4/4	0.92	0.18	28,37,37,42	0
5	EDO	C	1005	4/4	0.92	0.17	16,17,17,20	0
5	EDO	A	1009	4/4	0.93	0.20	17,18,18,19	0
5	EDO	B	1009	4/4	0.93	0.12	13,13,13,14	0
5	EDO	B	1007	4/4	0.94	0.13	18,19,20,22	0
4	ASN	A	1006	9/9	0.94	0.14	9,10,11,11	0
5	EDO	D	1004	4/4	0.95	0.11	17,17,19,19	0
4	ASN	D	1003	9/9	0.95	0.12	10,12,14,15	0
5	EDO	A	1008	4/4	0.95	0.15	14,15,16,17	0
4	ASN	C	1003	9/9	0.96	0.12	11,11,13,14	0
4	ASN	B	1006	9/9	0.96	0.10	10,12,14,14	0
2	CL	A	1003	1/1	0.96	0.06	21,21,21,21	0
2	CL	C	1001	1/1	0.97	0.06	19,19,19,19	0
5	EDO	C	1004	4/4	0.97	0.14	14,15,16,16	0
2	CL	D	1001	1/1	0.98	0.07	19,19,19,19	0
2	CL	B	1001	1/1	0.98	0.05	13,13,13,13	0
2	CL	A	1004	1/1	0.99	0.07	25,25,25,25	0
2	CL	B	1003	1/1	0.99	0.06	19,19,19,19	0
2	CL	A	1001	1/1	0.99	0.07	13,13,13,13	0
2	CL	A	1002	1/1	0.99	0.07	14,14,14,14	0
2	CL	B	1002	1/1	0.99	0.06	13,13,13,13	0
2	CL	B	1004	1/1	1.00	0.08	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.