Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:01 AM GMT

PDB ID	:	2P2N
Title	:	Crystal Structure and Allosteric Regulation of the Cytoplasmic Escherichia coli L-Asparaginase I
Authors	:	Yun, M.-K.; Nourse, A.; White, S.W.; Rock, C.O.; Heath, R.J.
Deposited on	:	2007-03-07
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

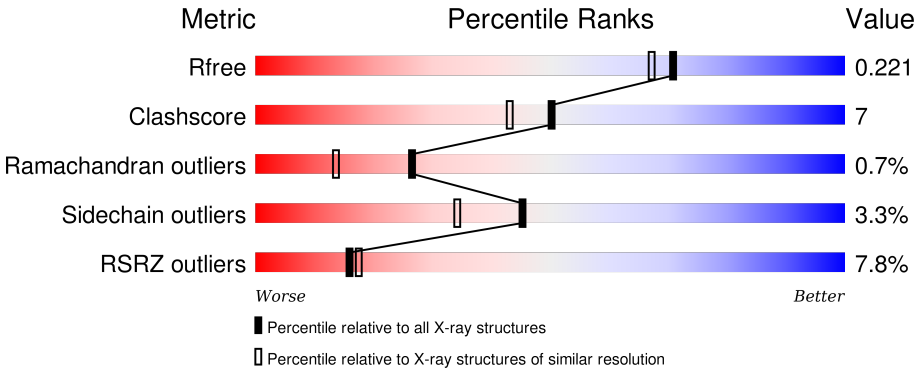
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (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. 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 <=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	6% 72% 12% • 15%
1	B	358	7% 76% 12% • 10%
1	C	358	9% 74% 11% • 14%
1	D	358	6% 76% 11% • 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
3	ASP	B	7003[A]	-	-	-	X
3	ASP	D	7007[A]	-	-	-	X
3	ASN	D	7008[B]	-	-	-	X
4	ASN	D	8004	-	-	-	X
5	EDO	A	9005	-	-	-	X
5	EDO	B	9004	-	-	-	X
5	EDO	C	9010	-	-	-	X
5	EDO	D	9007	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10323 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	304	Total	C	N	O	S	0	0	0
			2326	1476	396	444	10			
1	B	321	Total	C	N	O	S	0	0	0
			2464	1562	424	467	11			
1	C	307	Total	C	N	O	S	0	0	0
			2359	1500	401	447	11			
1	D	319	Total	C	N	O	S	0	0	0
			2440	1549	417	464	10			

There are 80 discrepancies between the modelled and reference sequences:

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

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

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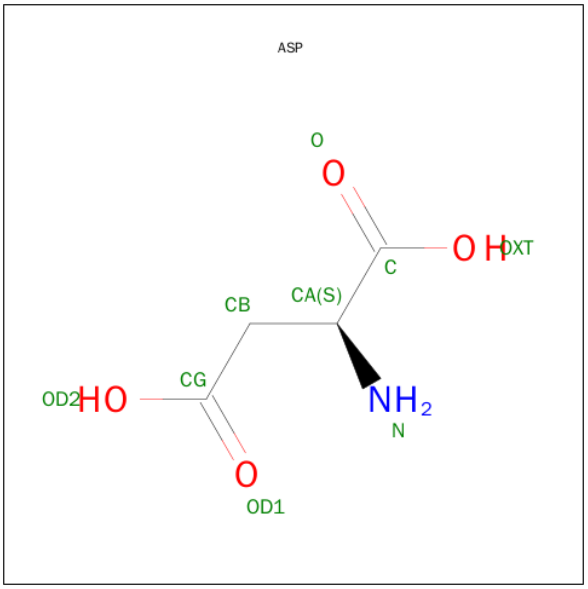
Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	CLONING ARTIFACT	UNP P0A962
D	-15	HIS	-	CLONING ARTIFACT	UNP P0A962
D	-14	HIS	-	CLONING ARTIFACT	UNP P0A962
D	-13	HIS	-	CLONING ARTIFACT	UNP P0A962
D	-12	HIS	-	CLONING ARTIFACT	UNP P0A962
D	-11	HIS	-	CLONING ARTIFACT	UNP P0A962
D	-10	HIS	-	CLONING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

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

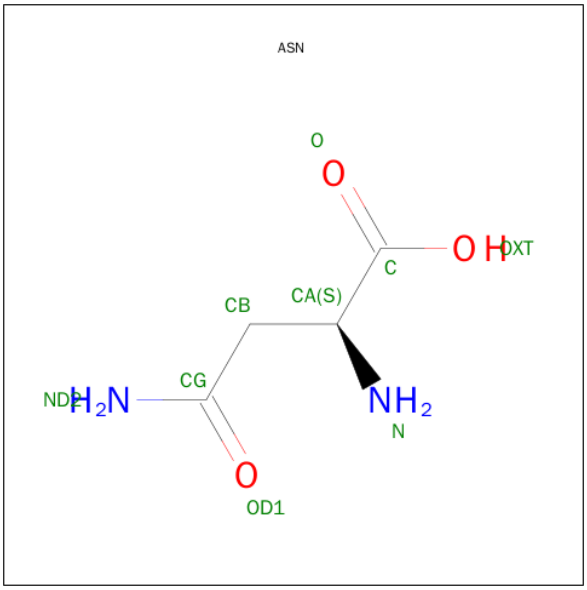
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Cl 2 2	0	0
2	A	2	Total Cl 2 2	0	0

- Molecule 3 is ASPARTIC ACID (three-letter code: ASP, ASN) (formula: $C_4H_7NO_4$, $C_4H_8N_2O_3$).



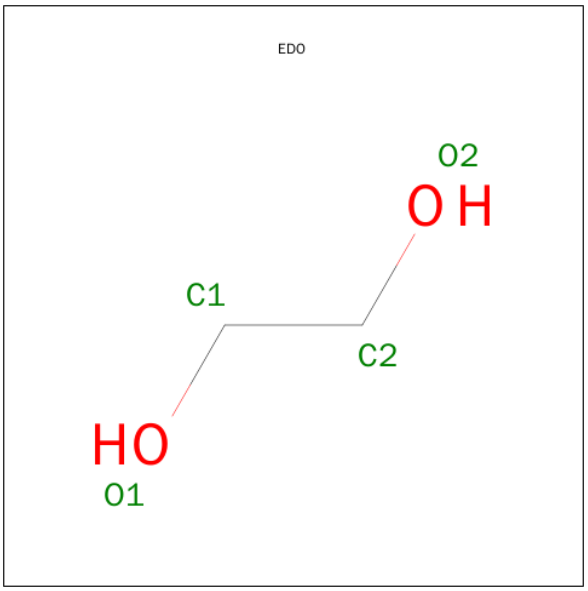
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total C N O 17 8 3 6	0	2
3	B	2	Total C N O 18 8 3 7	0	2
3	C	2	Total C N O 18 8 3 7	0	2
3	D	2	Total C N O 18 8 3 7	0	2

- 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 9 4 2 3	0	0
4	B	1	Total C N O 9 4 2 3	0	0
4	C	1	Total C N O 9 4 2 3	0	0
4	D	1	Total C N O 9 4 2 3	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is water.

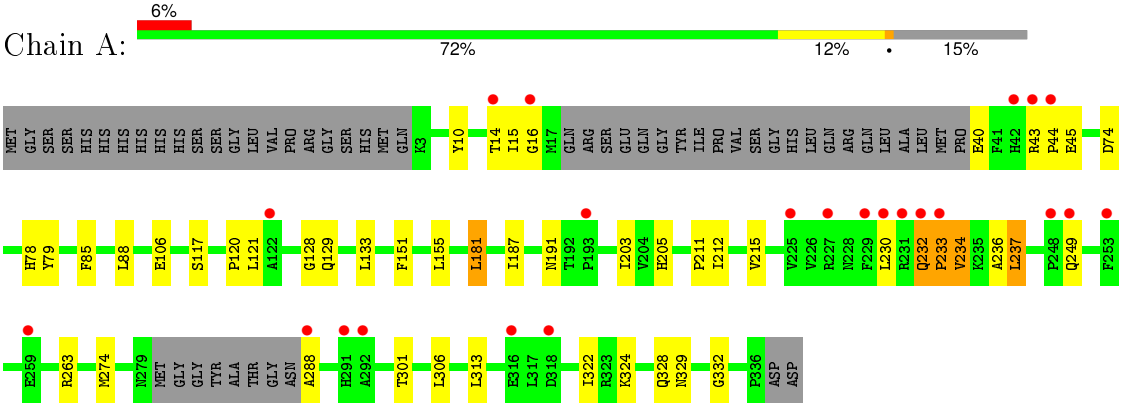
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	140	Total O 140 140	0	0
6	B	148	Total O 148 148	0	0
6	C	125	Total O 125 125	0	0
6	D	162	Total O 162 162	0	0

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 errors 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.

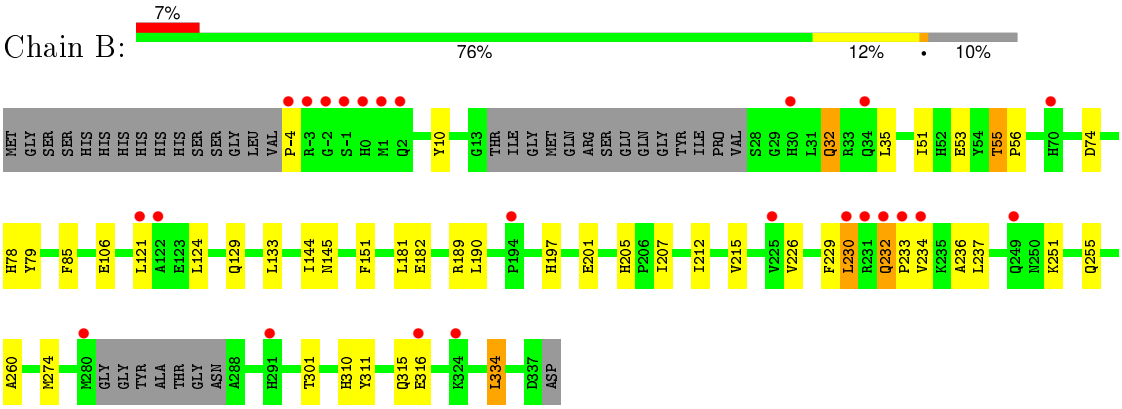
- Molecule 1: L-ASPARAGINASE I

Chain A:



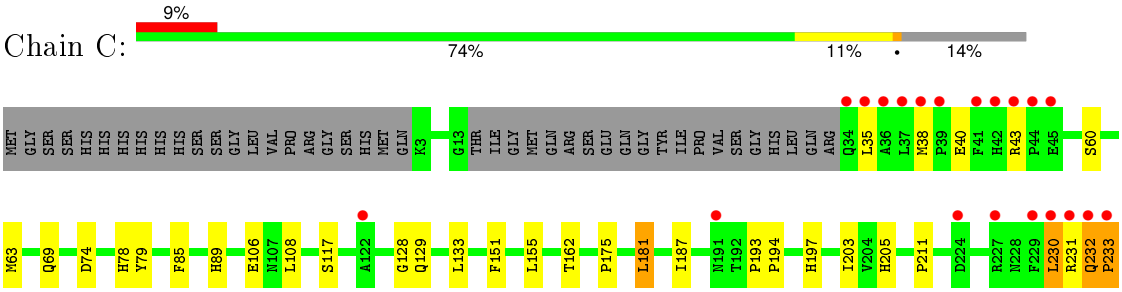
- Molecule 1: L-ASPARAGINASE I

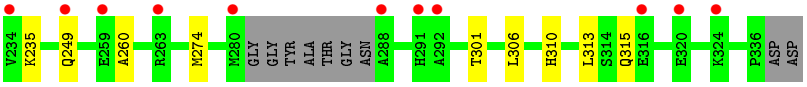
Chain B:



- Molecule 1: L-ASPARAGINASE I

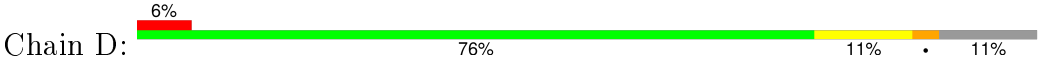
Chain C:

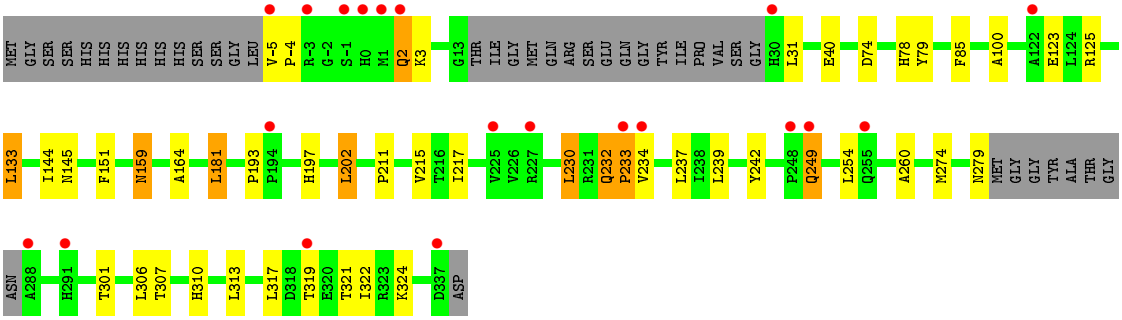




- Molecule 1: L-ASPARAGINASE I

Chain D:





4 Data and refinement statistics (i)

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)	50.00 – 1.90 45.13 – 1.89	Depositor EDS
% Data completeness (in resolution range)	90.7 (50.00-1.90) 90.3 (45.13-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	4.27 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.223 , 0.264 0.224 , 0.221	Depositor DCC
R_{free} test set	4749 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	19.4	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 57.4	EDS
Estimated twinning fraction	0.147 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 94998 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10323	wwPDB-VP
Average B, all atoms (Å^2)	19.0	wwPDB-VP

Xtriage'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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, CL

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	0.59	0/2377	0.66	2/3239 (0.1%)
1	B	0.59	0/2519	0.66	2/3429 (0.1%)
1	C	0.59	0/2411	0.64	1/3284 (0.0%)
1	D	0.60	0/2494	0.70	4/3399 (0.1%)
All	All	0.59	0/9801	0.67	9/13351 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	181	LEU	CA-CB-CG	7.12	131.68	115.30
1	A	181	LEU	CA-CB-CG	6.08	129.28	115.30
1	C	181	LEU	CA-CB-CG	5.92	128.92	115.30
1	B	334	LEU	CA-CB-CG	5.69	128.39	115.30
1	A	133	LEU	CA-CB-CG	5.55	128.07	115.30
1	D	133	LEU	CA-CB-CG	5.42	127.77	115.30
1	D	306	LEU	CA-CB-CG	5.34	127.57	115.30
1	B	181	LEU	CA-CB-CG	5.22	127.31	115.30
1	D	202	LEU	CA-CB-CG	5.20	127.26	115.30

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	2326	0	2276	35	0
1	B	2464	0	2424	30	0
1	C	2359	0	2327	34	0
1	D	2440	0	2393	41	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	17	0	8	0	0
3	B	18	0	8	0	0
3	C	18	0	8	0	0
3	D	18	0	8	0	0
4	A	9	0	5	1	0
4	B	9	0	5	0	0
4	C	9	0	5	3	0
4	D	9	0	5	0	0
5	A	8	0	12	2	0
5	B	12	0	18	1	0
5	C	8	0	12	1	0
5	D	20	0	30	1	0
6	A	140	0	0	1	0
6	B	148	0	0	1	0
6	C	125	0	0	2	0
6	D	162	0	0	2	0
All	All	10323	0	9544	135	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 (135) 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:C:232:GLN:H	1:C:233:PRO:HD3	1.17	1.00
1:A:232:GLN:H	1:A:233:PRO:HD3	1.23	0.97
1:C:232:GLN:N	1:C:233:PRO:HD3	1.90	0.85
1:A:232:GLN:H	1:A:233:PRO:CD	1.90	0.84
1:A:232:GLN:N	1:A:233:PRO:HD3	2.01	0.75
1:C:106:GLU:OE1	1:C:205:HIS:HE1	1.70	0.74
1:C:175:PRO:HG3	1:C:274:MET:HE2	1.71	0.72
1:A:10:TYR:OH	1:A:16:GLY:HA3	1.91	0.70
1:A:43:ARG:HB2	1:A:44:PRO:HD2	1.75	0.69
1:A:106:GLU:OE2	1:A:205:HIS:HE1	1.75	0.69
1:D:230:LEU:HD11	1:D:260:ALA:HA	1.75	0.68
1:C:232:GLN:H	1:C:233:PRO:CD	2.00	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:HIS:HD2	6:C:9107:HOH:O	1.76	0.68
1:A:301:THR:HA	5:A:9002:EDO:H12	1.75	0.68
1:C:274:MET:HE1	4:C:8003:ASN:HB3	1.77	0.66
1:D:232:GLN:H	1:D:233:PRO:CD	2.08	0.65
1:B:215:VAL:CG2	1:B:237:LEU:HD21	2.27	0.65
1:B:229:PHE:HB3	1:B:234:VAL:HG21	1.78	0.64
1:C:108:LEU:O	1:C:197:HIS:HE1	1.81	0.64
1:C:301:THR:HA	5:C:9001:EDO:H12	1.81	0.62
1:C:230:LEU:HD11	1:C:260:ALA:HA	1.80	0.62
1:C:74:ASP:O	1:C:78:HIS:HD2	1.83	0.61
1:A:324:LYS:O	1:A:328:GLN:HG3	2.01	0.60
1:D:249:GLN:HG3	1:D:254:LEU:HD11	1.83	0.60
1:D:215:VAL:HG12	1:D:239:LEU:HD23	1.83	0.59
1:C:38:MET:SD	1:C:129:GLN:HG2	2.42	0.59
1:B:233:PRO:O	1:B:234:VAL:HG23	2.02	0.59
1:C:232:GLN:N	1:C:233:PRO:CD	2.60	0.59
1:A:15:ILE:HD13	1:A:88:LEU:HD22	1.85	0.58
1:A:43:ARG:HD3	1:B:124:LEU:HD13	1.85	0.58
1:C:35:LEU:HA	1:C:38:MET:HE3	1.85	0.58
1:C:106:GLU:OE1	1:C:205:HIS:CE1	2.55	0.57
1:D:215:VAL:CG1	1:D:239:LEU:CD2	2.82	0.57
1:A:74:ASP:O	1:A:78:HIS:HD2	1.87	0.57
1:D:-5:VAL:HA	1:D:144:ILE:HG12	1.87	0.56
1:B:274:MET:CE	1:D:274:MET:HB2	2.35	0.56
1:A:106:GLU:OE2	1:A:205:HIS:CE1	2.57	0.56
1:B:207:ILE:HG23	1:B:310:HIS:HB3	1.88	0.55
1:B:79:TYR:HA	1:B:85:PHE:HZ	1.72	0.55
1:C:230:LEU:HD21	1:C:260:ALA:HB2	1.87	0.55
1:B:215:VAL:HG21	1:B:237:LEU:HD21	1.89	0.55
1:A:274:MET:HE1	6:C:9124:HOH:O	2.07	0.54
1:C:162:THR:HG21	1:C:274:MET:CE	2.37	0.54
1:C:60:SER:HB2	1:C:89:HIS:CE1	2.43	0.53
6:B:9031:HOH:O	1:D:310:HIS:HE1	1.91	0.53
1:C:274:MET:CE	4:C:8003:ASN:HB3	2.38	0.53
1:D:215:VAL:CG1	1:D:239:LEU:HD22	2.39	0.53
1:C:274:MET:HE1	4:C:8003:ASN:CB	2.39	0.52
1:D:40:GLU:HG3	1:D:133:LEU:HD23	1.92	0.52
1:D:319:THR:HG22	6:D:9116:HOH:O	2.09	0.52
1:A:329:ASN:HD21	1:A:332:GLY:CA	2.22	0.51
1:D:234:VAL:HG11	1:D:237:LEU:HD13	1.93	0.51
1:D:79:TYR:HA	1:D:85:PHE:CZ	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:MET:HE3	1:D:274:MET:HB2	1.92	0.51
1:D:313:LEU:HD23	1:D:322:ILE:HD13	1.91	0.51
1:A:40:GLU:O	1:A:43:ARG:HG2	2.11	0.51
1:B:226:VAL:O	1:B:230:LEU:HD23	2.11	0.51
1:B:215:VAL:HG23	1:B:237:LEU:HD21	1.92	0.50
1:D:215:VAL:HG11	1:D:239:LEU:HD22	1.93	0.50
1:D:-5:VAL:CB	1:D:144:ILE:HD11	2.41	0.50
1:A:249:GLN:NE2	1:A:288:ALA:HB3	2.27	0.50
1:B:79:TYR:HA	1:B:85:PHE:CZ	2.46	0.50
1:A:191:ASN:HD22	1:D:193:PRO:HD3	1.76	0.50
1:D:217:ILE:HG22	1:D:242:TYR:CZ	2.46	0.49
1:A:79:TYR:HA	1:A:85:PHE:CZ	2.46	0.49
1:D:211:PRO:HB2	1:D:233:PRO:C	2.33	0.49
1:A:232:GLN:N	1:A:233:PRO:CD	2.65	0.49
1:D:310:HIS:HD2	6:D:9138:HOH:O	1.95	0.49
1:D:301:THR:HA	5:D:9003:EDO:H21	1.94	0.49
1:D:79:TYR:HA	1:D:85:PHE:HZ	1.77	0.49
1:B:32:GLN:HE21	1:B:32:GLN:H	1.60	0.48
1:D:215:VAL:CG1	1:D:239:LEU:HD23	2.44	0.48
1:A:15:ILE:O	1:A:121:LEU:CB	2.62	0.47
1:B:145:ASN:HB2	1:B:197:HIS:HE1	1.79	0.47
1:D:159:ASN:HD22	1:D:159:ASN:C	2.18	0.47
1:D:211:PRO:HB2	1:D:233:PRO:O	2.13	0.47
1:B:121:LEU:HD11	1:B:129:GLN:HG3	1.96	0.47
1:B:230:LEU:HD11	1:B:260:ALA:HA	1.95	0.47
1:A:121:LEU:CB	1:A:129:GLN:HE22	2.28	0.46
1:C:235:LYS:HE2	1:C:313:LEU:HD22	1.97	0.46
1:B:121:LEU:CD1	1:B:129:GLN:HG3	2.46	0.46
1:C:211:PRO:HB2	1:C:233:PRO:O	2.15	0.46
1:A:234:VAL:HG11	1:A:237:LEU:HD23	1.98	0.46
1:A:45:GLU:HB2	1:B:124:LEU:HD22	1.97	0.46
1:D:215:VAL:HG11	1:D:239:LEU:CD2	2.46	0.46
1:A:313:LEU:HD23	1:A:322:ILE:HD13	1.97	0.46
1:C:274:MET:HE3	1:C:274:MET:O	2.16	0.46
1:B:230:LEU:HD21	1:B:260:ALA:HB2	1.96	0.46
1:C:40:GLU:HA	1:C:43:ARG:HG3	1.98	0.45
1:B:212:ILE:HG12	1:B:236:ALA:HB3	1.98	0.45
1:D:164:ALA:HB2	1:D:274:MET:HE1	1.98	0.45
1:D:74:ASP:O	1:D:78:HIS:HD2	1.99	0.45
1:C:106:GLU:HB3	1:C:203:ILE:HB	1.97	0.45
1:A:117:SER:HB3	1:A:128:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:GLN:H	1:D:233:PRO:HD3	1.82	0.45
1:D:-4:PRO:HD2	1:D:144:ILE:HG12	1.99	0.44
1:A:215:VAL:CG2	1:A:237:LEU:HD11	2.47	0.44
1:C:175:PRO:HG3	1:C:274:MET:CE	2.43	0.44
1:A:230:LEU:O	1:A:263:ARG:NH1	2.51	0.44
1:C:79:TYR:HA	1:C:85:PHE:CZ	2.52	0.44
1:D:145:ASN:HB2	1:D:197:HIS:HE1	1.82	0.44
1:B:232:GLN:O	1:B:234:VAL:N	2.43	0.44
1:B:301:THR:HA	5:B:9004:EDO:H21	2.00	0.44
1:A:181:LEU:HD21	1:A:187:ILE:HG23	2.00	0.44
4:A:8001:ASN:N	5:A:9002:EDO:HO1	2.15	0.43
1:C:155:LEU:HB3	1:C:181:LEU:HB3	2.00	0.43
1:B:106:GLU:OE2	1:B:205:HIS:NE2	2.44	0.43
6:A:9027:HOH:O	1:C:310:HIS:HE1	2.01	0.43
1:A:14:THR:HG23	1:A:120:PRO:HD3	2.01	0.43
1:A:211:PRO:HB2	1:A:233:PRO:O	2.19	0.43
1:C:60:SER:HA	1:C:63:MET:HG3	2.01	0.43
1:B:-4:PRO:HD2	1:B:144:ILE:HG12	2.01	0.42
1:B:311:TYR:O	1:B:315:GLN:HG2	2.19	0.42
1:C:117:SER:HB3	1:C:128:GLY:HA2	2.01	0.42
1:C:187:ILE:HD11	1:D:125:ARG:CZ	2.50	0.42
1:D:317:LEU:HD22	1:D:321:THR:HG21	2.02	0.42
1:B:55:THR:HA	1:B:56:PRO:HA	1.92	0.42
1:D:145:ASN:HB2	1:D:197:HIS:CE1	2.54	0.42
1:D:-5:VAL:HA	1:D:-4:PRO:HD2	1.90	0.41
1:A:215:VAL:HG23	1:A:237:LEU:CD1	2.50	0.41
1:A:155:LEU:HB3	1:A:181:LEU:HB3	2.02	0.41
1:A:212:ILE:HG12	1:A:236:ALA:HB3	2.01	0.41
1:B:35:LEU:HD12	1:B:51:ILE:HD11	2.02	0.41
1:C:193:PRO:HA	1:C:194:PRO:HD3	1.96	0.41
1:A:106:GLU:HB3	1:A:203:ILE:HB	2.01	0.41
1:D:100:ALA:HA	1:D:307:THR:HB	2.02	0.41
1:B:10:TYR:HB3	1:B:53:GLU:HA	2.02	0.41
1:D:2:GLN:HE21	1:D:2:GLN:HB2	1.62	0.41
1:D:164:ALA:HB2	1:D:274:MET:CE	2.51	0.41
1:A:215:VAL:HG23	1:A:237:LEU:HD11	2.03	0.41
1:D:249:GLN:HA	1:D:249:GLN:HE21	1.86	0.40
1:B:74:ASP:O	1:B:78:HIS:HD2	2.04	0.40
1:B:182:GLU:OE2	1:B:190:LEU:HD11	2.21	0.40
1:C:162:THR:HG21	1:C:274:MET:HE2	2.02	0.40
1:D:233:PRO:O	1:D:234:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	298/358 (83%)	289 (97%)	7 (2%)	2 (1%)	26 14
1	B	315/358 (88%)	305 (97%)	9 (3%)	1 (0%)	46 35
1	C	301/358 (84%)	290 (96%)	8 (3%)	3 (1%)	19 7
1	D	313/358 (87%)	304 (97%)	7 (2%)	2 (1%)	30 17
All	All	1227/1432 (86%)	1188 (97%)	31 (2%)	8 (1%)	26 14

All (8) Ramachandran outliers are listed below:

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

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	248/298 (83%)	244 (98%)	4 (2%)	70	66
1	B	264/298 (89%)	253 (96%)	11 (4%)	36	24
1	C	253/298 (85%)	246 (97%)	7 (3%)	51	41
1	D	260/298 (87%)	248 (95%)	12 (5%)	33	21
All	All	1025/1192 (86%)	991 (97%)	34 (3%)	45	34

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	PHE
1	A	234	VAL
1	A	237	LEU
1	A	306	LEU
1	B	32	GLN
1	B	55	THR
1	B	133	LEU
1	B	151	PHE
1	B	189	ARG
1	B	201	GLU
1	B	230	LEU
1	B	251	LYS
1	B	255	GLN
1	B	316	GLU
1	B	334	LEU
1	C	69	GLN
1	C	133	LEU
1	C	151	PHE
1	C	230	LEU
1	C	249	GLN
1	C	306	LEU
1	C	315	GLN
1	D	2	GLN
1	D	3	LYS
1	D	31	LEU
1	D	123	GLU
1	D	151	PHE
1	D	159	ASN
1	D	181	LEU
1	D	202	LEU
1	D	230	LEU
1	D	249	GLN
1	D	279	ASN

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Mol	Chain	Res	Type
1	D	324	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	78	HIS
1	A	129	GLN
1	A	191	ASN
1	A	205	HIS
1	A	328	GLN
1	A	329	ASN
1	B	32	GLN
1	B	78	HIS
1	B	145	ASN
1	B	152	ASN
1	B	197	HIS
1	B	249	GLN
1	B	258	GLN
1	B	310	HIS
1	C	78	HIS
1	C	186	HIS
1	C	197	HIS
1	C	205	HIS
1	C	249	GLN
1	C	258	GLN
1	C	310	HIS
1	D	2	GLN
1	D	78	HIS
1	D	129	GLN
1	D	159	ASN
1	D	249	GLN
1	D	279	ASN
1	D	310	HIS
1	D	315	GLN

5.3.3 RNA

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 28 ligands modelled in this entry, 4 are monoatomic - leaving 24 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	$\#\|Z\| > 2$
3	ASP	A	7001[A]	1	4,7,8	0.46	0	1,8,10	1.36	0
3	ASN	A	7002[B]	-	5,8,8	0.46	0	4,10,10	0.33	0
4	ASN	A	8001	-	5,8,8	0.21	0	4,10,10	0.28	0
5	EDO	A	9002	-	3,3,3	0.54	0	2,2,2	0.67	0
5	EDO	A	9005	-	3,3,3	0.59	0	2,2,2	0.92	0
3	ASP	B	7003[A]	-	2,8,8	0.20	0	0,10,10	0.00	-
3	ASN	B	7004[B]	-	5,8,8	0.22	0	4,10,10	0.25	0
4	ASN	B	8002	-	5,8,8	0.65	0	4,10,10	0.18	0
5	EDO	B	9004	-	3,3,3	0.41	0	2,2,2	0.53	0
5	EDO	B	9008	-	3,3,3	0.46	0	2,2,2	0.48	0
5	EDO	B	9009	-	3,3,3	0.54	0	2,2,2	0.95	0
3	ASP	C	7005[A]	-	2,8,8	0.22	0	0,10,10	0.00	-
3	ASN	C	7006[B]	-	5,8,8	0.29	0	4,10,10	0.25	0
4	ASN	C	8003	-	5,8,8	0.25	0	4,10,10	0.19	0
5	EDO	C	9001	-	3,3,3	0.50	0	2,2,2	0.75	0
5	EDO	C	9010	-	3,3,3	0.66	0	2,2,2	0.82	0
3	ASP	D	7007[A]	-	2,8,8	0.14	0	0,10,10	0.00	-
3	ASN	D	7008[B]	-	5,8,8	0.29	0	4,10,10	0.16	0
4	ASN	D	8004	-	5,8,8	0.55	0	4,10,10	0.11	0
5	EDO	D	9003	-	3,3,3	0.44	0	2,2,2	0.47	0
5	EDO	D	9006	-	3,3,3	0.60	0	2,2,2	0.07	0
5	EDO	D	9007	-	3,3,3	0.65	0	2,2,2	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	EDO	D	9011	-	3,3,3	0.64	0	2,2,2	0.16	0
5	EDO	D	9012	-	3,3,3	0.66	0	2,2,2	0.70	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ASP	A	7001[A]	1	-	0/3/7/8	0/0/0/0
3	ASN	A	7002[B]	-	-	0/4/8/8	0/0/0/0
4	ASN	A	8001	-	-	0/4/8/8	0/0/0/0
5	EDO	A	9002	-	-	0/1/1/1	0/0/0/0
5	EDO	A	9005	-	-	0/1/1/1	0/0/0/0
3	ASP	B	7003[A]	-	-	0/2/8/8	0/0/0/0
3	ASN	B	7004[B]	-	-	0/4/8/8	0/0/0/0
4	ASN	B	8002	-	-	0/4/8/8	0/0/0/0
5	EDO	B	9004	-	-	0/1/1/1	0/0/0/0
5	EDO	B	9008	-	-	0/1/1/1	0/0/0/0
5	EDO	B	9009	-	-	0/1/1/1	0/0/0/0
3	ASP	C	7005[A]	-	-	0/2/8/8	0/0/0/0
3	ASN	C	7006[B]	-	-	0/4/8/8	0/0/0/0
4	ASN	C	8003	-	-	0/4/8/8	0/0/0/0
5	EDO	C	9001	-	-	0/1/1/1	0/0/0/0
5	EDO	C	9010	-	-	0/1/1/1	0/0/0/0
3	ASP	D	7007[A]	-	-	0/2/8/8	0/0/0/0
3	ASN	D	7008[B]	-	-	0/4/8/8	0/0/0/0
4	ASN	D	8004	-	-	0/4/8/8	0/0/0/0
5	EDO	D	9003	-	-	0/1/1/1	0/0/0/0
5	EDO	D	9006	-	-	0/1/1/1	0/0/0/0
5	EDO	D	9007	-	-	0/1/1/1	0/0/0/0
5	EDO	D	9011	-	-	0/1/1/1	0/0/0/0
5	EDO	D	9012	-	-	0/1/1/1	0/0/0/0

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.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	8001	ASN	1	0
5	A	9002	EDO	2	0
5	B	9004	EDO	1	0
4	C	8003	ASN	3	0
5	C	9001	EDO	1	0
5	D	9003	EDO	1	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, 95^{th} 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	304/358 (84%)	0.48	23 (7%)	17	18	8, 17, 38, 48	0
1	B	321/358 (89%)	0.43	24 (7%)	17	19	8, 16, 37, 44	0
1	C	307/358 (85%)	0.55	31 (10%)	9	10	8, 17, 44, 59	0
1	D	319/358 (89%)	0.38	20 (6%)	23	26	7, 16, 35, 45	0
All	All	1251/1432 (87%)	0.46	98 (7%)	16	17	7, 17, 38, 59	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	233	PRO	9.9
1	D	233	PRO	9.8
1	C	39	PRO	8.7
1	C	37	LEU	7.2
1	D	122	ALA	6.6
1	B	1	MET	5.3
1	B	231	ARG	5.3
1	A	14	THR	5.3
1	D	1	MET	5.1
1	A	233	PRO	4.9
1	C	42	HIS	4.8
1	C	232	GLN	4.8
1	C	36	ALA	4.8
1	C	230	LEU	4.7
1	C	233	PRO	4.6
1	C	231	ARG	4.6
1	C	44	PRO	4.4
1	A	42	HIS	4.4
1	D	288	ALA	4.2
1	A	231	ARG	4.2
1	A	249	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	122	ALA	4.2
1	A	316	GLU	4.0
1	D	0	HIS	4.0
1	B	232	GLN	3.8
1	B	291	HIS	3.8
1	B	0	HIS	3.7
1	C	316	GLU	3.6
1	D	-1	SER	3.6
1	C	288	ALA	3.6
1	B	225	VAL	3.6
1	A	44	PRO	3.5
1	C	43	ARG	3.5
1	B	2	GLN	3.5
1	D	-5	VAL	3.5
1	A	227	ARG	3.5
1	A	292	ALA	3.5
1	B	234	VAL	3.4
1	D	2	GLN	3.4
1	A	232	GLN	3.3
1	C	122	ALA	3.2
1	A	43	ARG	3.1
1	B	194	PRO	3.1
1	B	30	HIS	3.0
1	A	225	VAL	3.0
1	D	234	VAL	3.0
1	A	16	GLY	3.0
1	C	249	GLN	2.9
1	A	229	PHE	2.9
1	C	229	PHE	2.9
1	D	-3	ARG	2.9
1	B	-3	ARG	2.8
1	C	227	ARG	2.8
1	B	-2	GLY	2.8
1	B	121	LEU	2.8
1	C	292	ALA	2.8
1	B	280	MET	2.8
1	C	35	LEU	2.7
1	D	291	HIS	2.7
1	A	253	PHE	2.7
1	D	249	GLN	2.7
1	C	234	VAL	2.7
1	C	259	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	38	MET	2.6
1	C	224	ASP	2.6
1	A	230	LEU	2.5
1	C	41	PHE	2.5
1	A	291	HIS	2.5
1	D	225	VAL	2.5
1	C	324	LYS	2.5
1	A	122	ALA	2.4
1	A	318	ASP	2.4
1	C	263	ARG	2.4
1	B	34	GLN	2.4
1	B	316	GLU	2.4
1	D	194	PRO	2.4
1	A	259	GLU	2.3
1	B	-1	SER	2.3
1	D	255	GLN	2.3
1	A	248	PRO	2.3
1	A	288	ALA	2.3
1	D	337	ASP	2.3
1	C	191	ASN	2.2
1	D	30	HIS	2.2
1	B	324	LYS	2.2
1	D	248	PRO	2.2
1	B	230	LEU	2.2
1	D	227	ARG	2.2
1	C	45	GLU	2.2
1	C	291	HIS	2.2
1	B	70	HIS	2.1
1	A	193	PRO	2.1
1	B	249	GLN	2.1
1	D	319	THR	2.1
1	C	280	MET	2.1
1	C	34	GLN	2.1
1	B	-4	PRO	2.0
1	C	320	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
3	ASP	D	7007[A]	9/9	0.77	0.20	3.78	6,12,13,13	9
5	EDO	A	9005	4/4	0.90	0.20	3.28	11,15,15,18	0
5	EDO	C	9010	4/4	0.89	0.18	2.76	12,13,14,17	0
5	EDO	B	9004	4/4	0.95	0.15	2.67	15,15,18,19	0
4	ASN	D	8004	9/9	0.94	0.14	2.45	7,9,12,12	0
3	ASP	B	7003[A]	9/9	0.76	0.20	2.37	8,14,15,15	9
3	ASN	D	7008[B]	9/9	0.87	0.16	2.27	10,12,12,12	9
5	EDO	D	9007	4/4	0.69	0.17	2.21	27,27,27,28	0
5	EDO	D	9003	4/4	0.94	0.12	1.91	14,15,16,17	0
5	EDO	D	9006	4/4	0.89	0.12	1.56	15,16,17,19	0
4	ASN	A	8001	9/9	0.93	0.14	1.45	5,8,10,10	0
4	ASN	C	8003	9/9	0.95	0.15	1.32	8,10,12,13	0
3	ASN	B	7004[B]	9/9	0.90	0.16	1.24	15,18,18,18	9
3	ASN	C	7006[B]	9/9	0.85	0.17	1.13	15,17,17,18	9
5	EDO	B	9009	4/4	0.94	0.12	1.11	10,11,12,16	0
5	EDO	D	9012	4/4	0.92	0.12	1.05	14,14,16,16	0
3	ASP	C	7005[A]	9/9	0.84	0.16	0.82	3,9,12,12	9
5	EDO	A	9002	4/4	0.96	0.13	0.65	7,9,12,13	0
3	ASN	A	7002[B]	9/9	0.80	0.18	0.58	14,16,17,17	9
3	ASP	A	7001[A]	8/9	0.77	0.18	0.56	9,17,17,18	8
4	ASN	B	8002	9/9	0.96	0.11	0.20	8,10,12,12	0
5	EDO	D	9011	4/4	0.80	0.13	-0.26	26,28,29,30	0
5	EDO	B	9008	4/4	0.85	0.16	-0.63	29,33,33,35	0
5	EDO	C	9001	4/4	0.96	0.09	-1.30	7,11,12,13	0
2	CL	B	1004	1/1	0.99	0.08	-1.57	13,13,13,13	0
2	CL	B	1003	1/1	0.99	0.06	-1.77	13,13,13,13	0
2	CL	A	1001	1/1	0.99	0.08	-2.17	13,13,13,13	0
2	CL	A	1002	1/1	0.99	0.07	-3.29	15,15,15,15	0

6.5 Other polymers (i)

There are no such residues in this entry.