



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2020 – 10:56 AM EST

PDB ID : 6P24
Title : Escherichia coli tRNA synthetase
Authors : Kahne, D.; Baidin, V.; Owens, T.W.
Deposited on : 2019-05-20
Resolution : 2.12 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 : 2.14.6
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) : 2.14.6

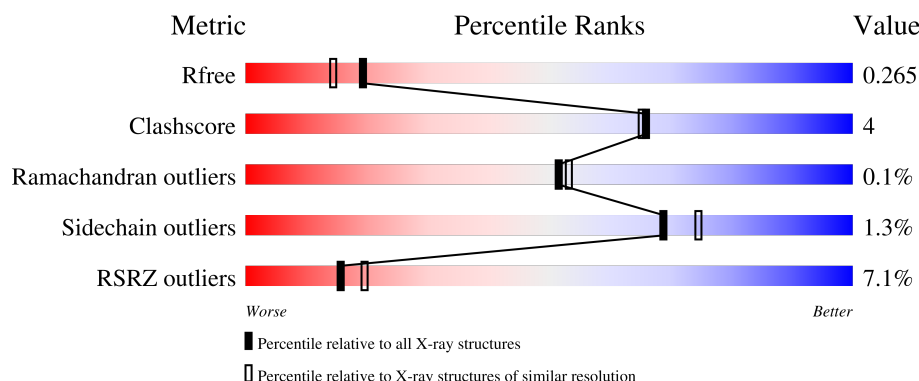
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.12 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	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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	332	<div> <div>5%</div> <div>63%</div> <div>10%</div> <div>27%</div> </div>
1	C	332	<div> <div>21%</div> <div>80%</div> <div>17%</div> <div>.</div> </div>
2	B	795	<div> <div>8%</div> <div>91%</div> <div>9%</div> </div>
2	D	795	<div> <div>%</div> <div>90%</div> <div>10%</div> </div>

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	MG	D	802	-	-	-	X
6	TRS	C	407	-	-	-	X
6	TRS	D	807	-	-	-	X
8	EDO	C	406	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 17272 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 Phenylalanine–tRNA ligase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	1	0
			1925	1227	337	352	9			
1	C	323	Total	C	N	O	S	0	0	0
			2447	1542	441	455	9			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP P08312
A	-3	SER	-	expression tag	UNP P08312
A	-2	HIS	-	expression tag	UNP P08312
A	-1	MET	-	expression tag	UNP P08312
A	0	ALA	-	expression tag	UNP P08312
A	1	SER	-	expression tag	UNP P08312
C	-4	GLY	-	expression tag	UNP P08312
C	-3	SER	-	expression tag	UNP P08312
C	-2	HIS	-	expression tag	UNP P08312
C	-1	MET	-	expression tag	UNP P08312
C	0	ALA	-	expression tag	UNP P08312
C	1	SER	-	expression tag	UNP P08312

- Molecule 2 is a protein called Phenylalanine–tRNA ligase beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	793	Total	C	N	O	S	0	0	0
			6041	3797	1061	1156	27			
2	D	794	Total	C	N	O	S	0	0	0
			6088	3832	1076	1153	27			

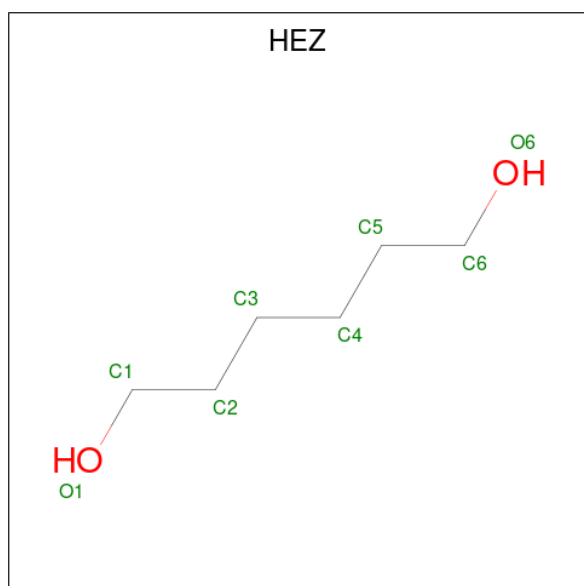
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	4	Total Mg 4 4	0	0
3	A	5	Total Mg 5 5	0	0
3	D	2	Total Mg 2 2	0	0
3	C	2	Total Mg 2 2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

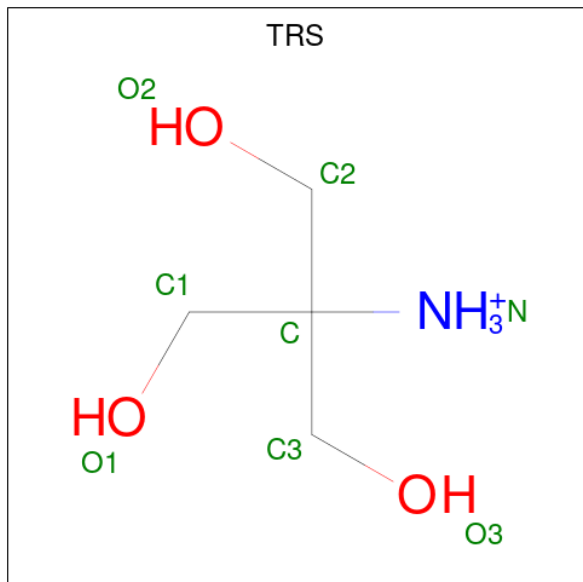
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0

- Molecule 5 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 8 6 2	0	0
5	D	1	Total C O 8 6 2	0	0
5	D	1	Total C O 8 6 2	0	0
5	D	1	Total C O 8 6 2	0	0
5	D	1	Total C O 8 6 2	0	0

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			8	4	1	3		
6	A	1	Total	C	N	O	0	0
			8	4	1	3		
6	C	1	Total	C	N	O	0	0
			8	4	1	3		
6	D	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	0
			7	4	3		
7	B	1	Total	C	O	0	0
			7	4	3		
7	C	1	Total	C	O	0	0
			7	4	3		
7	C	1	Total	C	O	0	0
			7	4	3		
7	D	1	Total	C	O	0	0
			7	4	3		
7	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



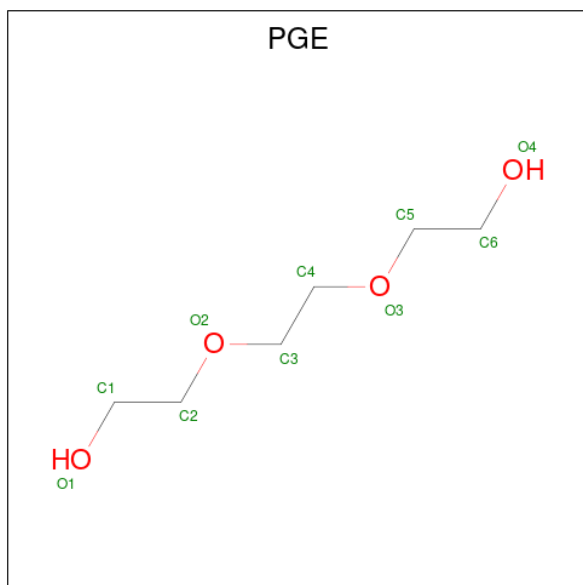
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	B	1	Total	C	O	0	0
			4	2	2		
8	C	1	Total	C	O	0	0
			4	2	2		
8	C	1	Total	C	O	0	0
			4	2	2		
8	C	1	Total	C	O	0	0
			4	2	2		
8	D	1	Total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

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

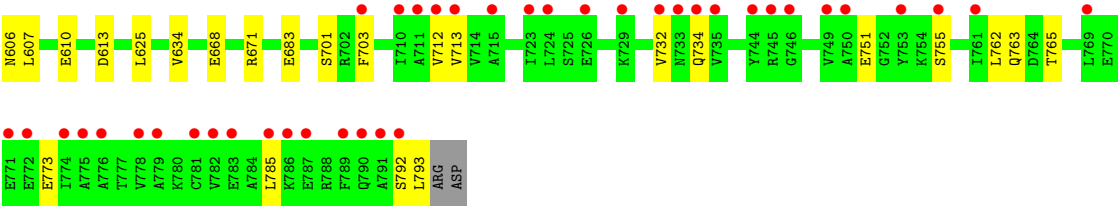
- Molecule 9 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



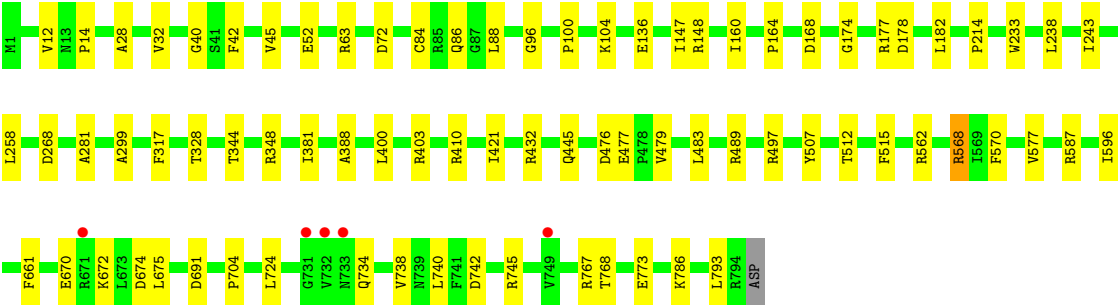
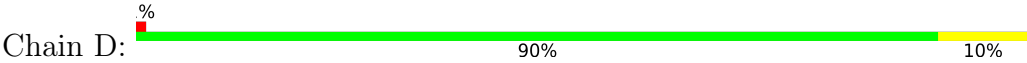
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			10	6	4		
9	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	56	Total	O	0	0
			56	56		
10	B	169	Total	O	0	0
			169	169		
10	C	46	Total	O	0	0
			46	46		
10	D	256	Total	O	0	0
			256	256		



● Molecule 2: Phenylalanine-tRNA ligase beta subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.27Å 173.58Å 251.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	82.04 – 2.12 82.04 – 2.12	Depositor EDS
% Data completeness (in resolution range)	99.1 (82.04-2.12) 99.1 (82.04-2.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.12Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, R_{free}	0.229 , 0.265 0.229 , 0.265	Depositor DCC
R_{free} test set	1994 reflections (1.31%)	wwPDB-VP
Wilson B-factor (Å ²)	50.9	Xtriage
Anisotropy	0.148	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17272	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.23% 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: MG, PGE, CL, EDO, HEZ, TRS, PEG

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	0.25	0/1979	0.42	0/2684
1	C	0.24	0/2503	0.40	0/3402
2	B	0.24	0/6142	0.42	0/8350
2	D	0.24	0/6190	0.44	0/8408
All	All	0.24	0/16814	0.42	0/22844

There are no bond length outliers.

There are no bond angle outliers.

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	1925	0	1829	22	0
1	C	2447	0	2281	35	0
2	B	6041	0	6019	46	0
2	D	6088	0	6122	46	0
3	A	5	0	0	0	0
3	B	4	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	8	0	14	0	0
5	D	32	0	56	2	0
6	A	16	0	24	3	0
6	C	8	0	12	1	0
6	D	8	0	12	0	0
7	A	7	0	10	0	0
7	B	35	0	50	3	0
7	C	14	0	20	2	0
7	D	14	0	20	1	0
8	A	4	0	6	0	0
8	B	16	0	24	4	0
8	C	12	0	18	0	0
8	D	36	0	54	1	0
9	B	20	0	28	1	0
10	A	56	0	0	1	0
10	B	169	0	0	2	0
10	C	46	0	0	1	0
10	D	256	0	0	4	0
All	All	17272	0	16599	133	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 4.

All (133) 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)
2:D:28:ALA:HB2	2:D:182:LEU:HD11	1.63	0.81
2:B:40:GLY:O	2:B:148:ARG:NH2	2.21	0.72
2:B:604:HIS:HA	8:B:814:EDO:H21	1.70	0.71
2:B:497:ARG:HH21	7:C:404:PEG:H32	1.58	0.68
1:C:324:LYS:HG3	1:C:327:LYS:HE2	1.74	0.68
1:C:228:HIS:ND1	2:D:476:ASP:OD2	2.26	0.68
1:A:169:GLN:NE2	10:A:502:HOH:O	2.27	0.68
2:B:129:ASP:OD2	2:B:244:ARG:NH2	2.27	0.68
2:B:606:ASN:HD21	8:B:815:EDO:H11	1.58	0.67
1:C:42:MET:HA	1:C:60:ILE:HD13	1.77	0.67
6:A:408:TRS:H31	2:D:497:ARG:HH21	1.60	0.66
1:A:227:LEU:HD13	1:A:270:LEU:HD11	1.80	0.64
2:D:177:ARG:NH1	10:D:904:HOH:O	2.30	0.62
1:C:192:ARG:NH2	2:D:512:THR:O	2.34	0.61
2:B:237:LYS:NZ	10:B:910:HOH:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:MET:HG2	1:C:185:ILE:HD13	1.83	0.59
1:A:222:ASN:HB3	2:B:479:VAL:HG22	1.85	0.58
2:D:63:ARG:NH1	2:D:84:CYS:O	2.37	0.58
2:D:40:GLY:O	2:D:148:ARG:NH2	2.38	0.57
1:A:105:GLY:HA2	6:A:408:TRS:H22	1.88	0.56
1:A:269:VAL:HG13	1:A:302:LEU:HD21	1.86	0.56
1:C:222:ASN:HB3	2:D:479:VAL:HG22	1.86	0.56
1:A:97:PRO:HB3	6:A:411:TRS:H12	1.87	0.56
2:D:568:ARG:HB3	2:D:596:ILE:HG22	1.89	0.55
1:C:156:ASP:HB3	1:C:196:ASN:HB3	1.88	0.55
1:C:195:ARG:HE	1:C:206:PHE:HZ	1.53	0.55
2:B:439:GLU:OE1	8:B:807:EDO:O2	2.23	0.55
2:D:489:ARG:NH2	2:D:691:ASP:OD1	2.40	0.55
1:C:257:VAL:HB	1:C:270:LEU:HB2	1.90	0.54
2:B:359:ARG:HH22	9:B:806:PGE:H22	1.73	0.54
1:C:15:ILE:HA	1:C:34:LYS:HE3	1.90	0.53
2:D:734:GLN:NE2	2:D:773:GLU:OE2	2.40	0.53
2:B:12:VAL:HG22	2:B:14:PRO:HD3	1.91	0.53
2:B:668:GLU:OE2	2:B:671:ARG:NH1	2.42	0.53
2:B:38:VAL:HG13	2:B:239:ARG:HH22	1.74	0.52
1:A:211:GLY:HA3	1:A:295:PHE:CZ	2.45	0.52
2:B:734:GLN:HB3	2:B:762:LEU:HD23	1.92	0.52
2:B:703:PHE:O	2:B:763:GLN:NE2	2.34	0.52
2:D:45:VAL:HB	2:D:147:ILE:HD11	1.91	0.51
1:A:219:SER:HG	1:A:221:THR:HG1	1.59	0.51
1:C:132:GLU:OE1	1:C:194:TYR:OH	2.23	0.51
2:B:138:PRO:HG2	7:B:810:PEG:H11	1.91	0.51
2:B:410:ARG:NH2	2:B:421:ILE:O	2.36	0.51
2:B:81:ALA:HB2	7:B:812:PEG:H41	1.94	0.50
1:C:148:HIS:HB2	2:D:344:THR:HG21	1.91	0.50
2:B:45:VAL:HB	2:B:147:ILE:HD11	1.93	0.50
2:B:445:GLN:NE2	10:B:904:HOH:O	2.45	0.50
1:A:132:GLU:OE1	1:A:194:TYR:OH	2.19	0.49
2:D:767:ARG:NH2	2:D:773:GLU:OE2	2.42	0.49
2:B:485:MET:HG2	1:C:123:LEU:HD11	1.94	0.49
2:D:168:ASP:O	2:D:174:GLY:HA3	2.12	0.49
1:A:99:ARG:HG3	2:B:607:LEU:HD21	1.95	0.49
1:A:123:LEU:HG	2:D:483:LEU:HB3	1.94	0.49
2:D:704:PRO:HD2	2:D:768:THR:HG22	1.94	0.49
1:C:112:THR:HG22	1:C:299:MET:HE3	1.96	0.48
2:D:243:ILE:HD12	2:D:258:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:233:TRP:HB3	5:D:806:HEZ:H52	1.95	0.48
2:D:52:GLU:HA	2:D:86:GLN:HG3	1.96	0.48
2:D:96:GLY:HA2	2:D:104:LYS:HE2	1.94	0.48
1:C:6:GLU:O	1:C:8:VAL:N	2.41	0.48
1:A:244:ARG:NH1	1:A:256:GLU:OE1	2.47	0.48
2:D:562:ARG:NH1	10:D:920:HOH:O	2.46	0.48
1:C:137:TYR:HA	1:C:141:ASP:HB2	1.96	0.47
1:C:224:LYS:NZ	2:D:476:ASP:OD1	2.47	0.47
2:D:577:VAL:HG23	2:D:587:ARG:HB3	1.96	0.47
1:A:156:ASP:HB3	1:A:196:ASN:H	1.80	0.47
2:D:42:PHE:HB3	2:D:100:PRO:HD3	1.97	0.47
1:A:92:ILE:HA	5:D:803:HEZ:H51	1.97	0.46
1:C:211:GLY:HA3	1:C:295:PHE:CZ	2.50	0.46
2:B:439:GLU:HB3	8:B:807:EDO:H22	1.97	0.46
1:C:186:ARG:O	6:C:407:TRS:H21	2.15	0.46
2:B:701:SER:HB2	2:B:765:THR:HA	1.97	0.46
1:C:247:TYR:CE2	2:D:164:PRO:HG2	2.50	0.46
1:C:144:ASN:HD21	1:C:278:ASN:HD22	1.64	0.46
1:C:281:ARG:NH1	10:C:510:HOH:O	2.48	0.46
2:B:604:HIS:HB3	2:B:607:LEU:HB2	1.97	0.46
1:C:232:ARG:NH1	1:C:238:ASP:OD1	2.48	0.46
1:C:104:GLY:HA3	2:D:507:TYR:O	2.16	0.46
2:B:712:VAL:HG11	2:B:785:LEU:HD23	1.97	0.45
2:D:670:GLU:HA	2:D:675:LEU:HD12	1.99	0.44
2:B:155:ASP:OD1	2:B:156:ASN:N	2.50	0.44
2:B:593:ALA:HB2	2:B:683:GLU:HG3	2.00	0.44
2:B:792:SER:OG	2:B:793:LEU:N	2.51	0.44
2:D:672:LYS:C	2:D:674:ASP:H	2.21	0.44
2:B:600:ARG:NH1	2:B:610:GLU:OE1	2.51	0.44
2:D:12:VAL:HG22	2:D:14:PRO:HD3	2.00	0.44
2:D:738:VAL:H	7:D:815:PEG:H22	1.83	0.44
1:A:269:VAL:HG12	1:A:270:LEU:HD23	2.00	0.44
2:B:128:SER:OG	2:B:129:ASP:N	2.51	0.44
2:B:625:LEU:HD13	2:B:634:VAL:HG11	2.00	0.44
1:C:74:ARG:NH1	1:C:77:GLU:OE1	2.46	0.44
2:D:410:ARG:NH2	2:D:421:ILE:O	2.43	0.44
2:D:507:TYR:HB3	2:D:570:PHE:HD2	1.83	0.43
2:D:72:ASP:N	2:D:72:ASP:OD1	2.50	0.43
1:C:112:THR:HG23	1:C:234:PHE:CE2	2.52	0.43
2:B:507:TYR:HB3	2:B:570:PHE:HD2	1.84	0.43
2:B:613:ASP:OD1	1:C:99:ARG:NH1	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:203:LEU:HD21	2:B:332:LEU:HD13	2.00	0.43
2:B:485:MET:HE1	1:C:230:PHE:HA	2.00	0.43
2:B:497:ARG:HE	7:C:404:PEG:H21	1.84	0.43
2:D:32:VAL:HG22	2:D:160:ILE:HG22	2.00	0.43
2:B:341:LEU:H	2:B:341:LEU:HD12	1.83	0.43
2:D:724:LEU:HD21	2:D:740:LEU:HB2	1.99	0.43
2:D:281:ALA:O	2:D:299:ALA:HA	2.19	0.43
2:B:311:LEU:HD22	2:B:322:SER:HB3	2.01	0.43
2:B:147:ILE:H	2:B:147:ILE:HG13	1.56	0.42
1:C:155:HIS:HB3	1:C:168:THR:HG21	2.01	0.42
1:A:224:LYS:HA	1:A:243:PHE:CZ	2.55	0.42
1:C:49:PRO:HA	1:C:50:PRO:HD3	1.96	0.42
2:D:704:PRO:HG2	8:D:812:EDO:H11	2.02	0.42
1:A:223:LEU:HD11	1:A:272:CYS:HB2	2.01	0.42
2:B:42:PHE:HB3	2:B:100:PRO:HD3	2.02	0.42
2:B:232:LEU:HB3	7:B:810:PEG:H12	2.02	0.42
1:C:133:ILE:HG12	1:C:166:LEU:HD23	2.02	0.42
2:D:403:ARG:NH2	10:D:915:HOH:O	2.44	0.42
1:A:222:ASN:HA	2:B:477:GLU:O	2.19	0.42
2:B:16:ILE:HB	2:B:20:ALA:HB3	2.01	0.41
2:D:88:LEU:HD21	2:D:136:GLU:HG2	2.01	0.41
2:D:214:PRO:HB2	2:D:400:LEU:HD23	2.03	0.41
2:D:268:ASP:OD1	2:D:328:THR:OG1	2.27	0.41
2:D:432:ARG:NH1	10:D:929:HOH:O	2.53	0.41
1:A:244:ARG:NH2	1:A:258:ASP:OD2	2.44	0.41
2:B:713:VAL:HA	2:B:755:SER:HA	2.03	0.41
2:B:168:ASP:O	2:B:174:GLY:HA3	2.21	0.41
1:A:104:GLY:HA3	2:B:507:TYR:O	2.21	0.41
1:C:222:ASN:HA	2:D:477:GLU:O	2.21	0.41
1:A:158:PHE:CZ	1:A:196:ASN:HA	2.56	0.40
1:C:112:THR:HG23	1:C:234:PHE:HE2	1.85	0.40
1:A:209:MET:HE3	1:A:209:MET:HB2	1.98	0.40
2:D:381:ILE:HD11	2:D:388:ALA:HB2	2.03	0.40
1:C:322:PHE:HA	1:C:325:GLN:HE21	1.85	0.40
1:C:218:ILE:HG21	1:C:292:GLY:HA2	2.04	0.40
2:D:786:LYS:HB2	2:D:786:LYS:HE3	1.84	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	240/332 (72%)	230 (96%)	10 (4%)	0	100	100
1	C	321/332 (97%)	305 (95%)	15 (5%)	1 (0%)	41	40
2	B	791/795 (100%)	771 (98%)	19 (2%)	1 (0%)	51	53
2	D	792/795 (100%)	773 (98%)	19 (2%)	0	100	100
All	All	2144/2254 (95%)	2079 (97%)	63 (3%)	2 (0%)	51	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	732	VAL
1	C	199	ASP

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	202/279 (72%)	199 (98%)	3 (2%)	65	70
1	C	238/279 (85%)	235 (99%)	3 (1%)	69	74
2	B	642/663 (97%)	637 (99%)	5 (1%)	81	86
2	D	651/663 (98%)	640 (98%)	11 (2%)	60	66
All	All	1733/1884 (92%)	1711 (99%)	22 (1%)	69	74

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	VAL
1	A	198	TYR
1	A	312	LEU
2	B	178	ASP
2	B	317	PHE
2	B	515	PHE
2	B	751	GLU
2	B	773	GLU
1	C	165	LEU
1	C	198	TYR
1	C	201	THR
2	D	178	ASP
2	D	238	LEU
2	D	317	PHE
2	D	348	ARG
2	D	445	GLN
2	D	515	PHE
2	D	568	ARG
2	D	661	PHE
2	D	742	ASP
2	D	745	ARG
2	D	793	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	144	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 52 ligands modelled in this entry, 14 are monoatomic - leaving 38 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	HEZ	D	803	-	7,7,7	0.31	0	6,6,6	0.88	0
7	PEG	B	811	-	6,6,6	0.68	0	5,5,5	0.59	0
6	TRS	A	411	-	7,7,7	0.30	0	9,9,9	0.27	0
8	EDO	D	809	-	3,3,3	0.45	0	2,2,2	0.38	0
8	EDO	D	811	-	3,3,3	0.48	0	2,2,2	0.27	0
8	EDO	B	815	-	3,3,3	0.45	0	2,2,2	0.35	0
7	PEG	C	404	-	6,6,6	0.71	0	5,5,5	0.56	0
5	HEZ	D	804	-	7,7,7	0.34	0	6,6,6	0.89	0
8	EDO	C	406	3	3,3,3	0.47	0	2,2,2	0.32	0
8	EDO	D	810	-	3,3,3	0.47	0	2,2,2	0.32	0
9	PGE	B	813	-	9,9,9	0.31	0	8,8,8	0.28	0
8	EDO	B	814	-	3,3,3	0.47	0	2,2,2	0.24	0
5	HEZ	D	805	-	7,7,7	0.32	0	6,6,6	0.91	0
5	HEZ	D	806	-	7,7,7	0.35	0	6,6,6	0.86	0
8	EDO	D	817	-	3,3,3	0.46	0	2,2,2	0.34	0
8	EDO	D	812	-	3,3,3	0.46	0	2,2,2	0.31	0
8	EDO	D	816	-	3,3,3	0.47	0	2,2,2	0.29	0
8	EDO	C	408	-	3,3,3	0.48	0	2,2,2	0.33	0
7	PEG	D	815	-	6,6,6	0.71	0	5,5,5	0.56	0
7	PEG	B	809	-	6,6,6	0.70	0	5,5,5	0.57	0
6	TRS	D	807	-	7,7,7	0.31	0	9,9,9	0.29	0
5	HEZ	A	407	-	7,7,7	0.33	0	6,6,6	0.89	0
8	EDO	D	808	-	3,3,3	0.44	0	2,2,2	0.42	0
8	EDO	B	808	-	3,3,3	0.45	0	2,2,2	0.36	0
7	PEG	A	409	-	6,6,6	0.69	0	5,5,5	0.58	0
6	TRS	C	407	-	7,7,7	0.30	0	9,9,9	0.31	0
8	EDO	D	818	-	3,3,3	0.46	0	2,2,2	0.36	0
7	PEG	C	405	-	6,6,6	0.70	0	5,5,5	0.55	0
7	PEG	D	813	-	6,6,6	0.70	0	5,5,5	0.54	0
8	EDO	D	814	-	3,3,3	0.47	0	2,2,2	0.34	0
8	EDO	C	403	-	3,3,3	0.45	0	2,2,2	0.30	0
7	PEG	B	810	-	6,6,6	0.70	0	5,5,5	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	EDO	B	807	-	3,3,3	0.44	0	2,2,2	0.37	0
8	EDO	A	410	-	3,3,3	0.45	0	2,2,2	0.37	0
9	PGE	B	806	-	9,9,9	0.32	0	8,8,8	0.25	0
6	TRS	A	408	-	7,7,7	0.29	0	9,9,9	0.25	0
7	PEG	B	805	-	6,6,6	0.68	0	5,5,5	0.55	0
7	PEG	B	812	-	6,6,6	0.71	0	5,5,5	0.55	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
5	HEZ	D	803	-	-	0/5/5/5	-
7	PEG	B	811	-	-	1/4/4/4	-
6	TRS	A	411	-	-	0/9/9/9	-
8	EDO	D	809	-	-	0/1/1/1	-
8	EDO	D	811	-	-	0/1/1/1	-
8	EDO	B	815	-	-	0/1/1/1	-
7	PEG	C	404	-	-	1/4/4/4	-
5	HEZ	D	804	-	-	4/5/5/5	-
8	EDO	C	406	3	-	1/1/1/1	-
8	EDO	D	810	-	-	0/1/1/1	-
9	PGE	B	813	-	-	4/7/7/7	-
8	EDO	B	814	-	-	0/1/1/1	-
5	HEZ	D	805	-	-	1/5/5/5	-
5	HEZ	D	806	-	-	3/5/5/5	-
8	EDO	D	817	-	-	0/1/1/1	-
8	EDO	D	812	-	-	0/1/1/1	-
8	EDO	D	816	-	-	0/1/1/1	-
8	EDO	C	408	-	-	0/1/1/1	-
7	PEG	D	815	-	-	0/4/4/4	-
7	PEG	B	809	-	-	2/4/4/4	-
6	TRS	D	807	-	-	0/9/9/9	-
5	HEZ	A	407	-	-	4/5/5/5	-
8	EDO	D	808	-	-	0/1/1/1	-
8	EDO	B	808	-	-	0/1/1/1	-
7	PEG	A	409	-	-	1/4/4/4	-
6	TRS	C	407	-	-	0/9/9/9	-
8	EDO	D	818	-	-	0/1/1/1	-
7	PEG	C	405	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PEG	D	813	-	-	1/4/4/4	-
8	EDO	D	814	-	-	0/1/1/1	-
8	EDO	C	403	-	-	0/1/1/1	-
7	PEG	B	810	-	-	0/4/4/4	-
8	EDO	B	807	-	-	0/1/1/1	-
8	EDO	A	410	-	-	0/1/1/1	-
9	PGE	B	806	-	-	1/7/7/7	-
6	TRS	A	408	-	-	2/9/9/9	-
7	PEG	B	805	-	-	3/4/4/4	-
7	PEG	B	812	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	408	TRS	N-C-C2-O2
7	C	405	PEG	O2-C3-C4-O4
5	D	804	HEZ	C2-C3-C4-C5
5	A	407	HEZ	C1-C2-C3-C4
5	D	806	HEZ	C1-C2-C3-C4
5	D	804	HEZ	C1-C2-C3-C4
7	B	811	PEG	O2-C3-C4-O4
5	D	806	HEZ	O1-C1-C2-C3
5	A	407	HEZ	O1-C1-C2-C3
9	B	813	PGE	O1-C1-C2-O2
5	D	804	HEZ	C4-C5-C6-O6
5	D	804	HEZ	C3-C4-C5-C6
7	B	809	PEG	O2-C3-C4-O4
8	C	406	EDO	O1-C1-C2-O2
7	D	813	PEG	C4-C3-O2-C2
7	B	805	PEG	C1-C2-O2-C3
7	C	405	PEG	C1-C2-O2-C3
9	B	806	PGE	O3-C5-C6-O4
5	A	407	HEZ	C2-C3-C4-C5
7	B	809	PEG	C4-C3-O2-C2
5	D	805	HEZ	C1-C2-C3-C4
7	C	404	PEG	C1-C2-O2-C3
9	B	813	PGE	C6-C5-O3-C4

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Mol	Chain	Res	Type	Atoms
9	B	813	PGE	C3-C4-O3-C5
9	B	813	PGE	C4-C3-O2-C2
7	A	409	PEG	O2-C3-C4-O4
7	B	812	PEG	O1-C1-C2-O2
7	B	805	PEG	C4-C3-O2-C2
6	A	408	TRS	C3-C-C2-O2
5	D	806	HEZ	C3-C4-C5-C6
5	A	407	HEZ	C4-C5-C6-O6
7	B	805	PEG	O2-C3-C4-O4

There are no ring outliers.

14 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	803	HEZ	1	0
6	A	411	TRS	1	0
8	B	815	EDO	1	0
7	C	404	PEG	2	0
8	B	814	EDO	1	0
5	D	806	HEZ	1	0
8	D	812	EDO	1	0
7	D	815	PEG	1	0
6	C	407	TRS	1	0
7	B	810	PEG	2	0
8	B	807	EDO	2	0
9	B	806	PGE	1	0
6	A	408	TRS	2	0
7	B	812	PEG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	241/332 (72%)	0.58	17 (7%) 16 19	37, 53, 94, 110	0
1	C	323/332 (97%)	1.28	70 (21%) 0 0	39, 63, 146, 157	0
2	B	793/795 (99%)	0.47	61 (7%) 13 17	40, 60, 97, 118	0
2	D	794/795 (99%)	0.18	5 (0%) 89 91	33, 53, 75, 91	0
All	All	2151/2254 (95%)	0.50	153 (7%) 16 19	33, 57, 102, 157	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	43	THR	12.0
2	B	787	GLU	10.4
2	B	791	ALA	9.7
1	C	46	ARG	9.3
1	C	40	LEU	8.7
1	C	5	ALA	7.9
1	A	153	ALA	7.7
1	C	42	MET	7.6
1	C	57	GLY	7.5
1	C	39	THR	7.2
1	C	49	PRO	6.9
1	C	31	TYR	6.7
1	C	60	ILE	6.6
1	C	63	ALA	6.5
1	A	201	THR	6.3
1	C	13	ALA	6.1
1	C	21	VAL	6.0
2	B	746	GLY	6.0
1	A	198	TYR	5.9
1	C	7	LEU	5.9
1	C	29	VAL	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	200	GLN	5.6
1	C	32	LEU	5.6
1	C	198	TYR	5.6
1	C	11	ALA	5.6
1	A	151	ALA	5.4
1	C	54	PRO	5.4
1	A	199	ASP	5.4
1	C	23	ALA	5.4
1	C	59	VAL	5.3
1	C	51	GLU	5.2
2	B	782	VAL	5.1
1	C	22	ALA	5.1
1	C	38	LEU	4.9
2	B	785	LEU	4.8
1	C	45	LEU	4.8
1	A	155	HIS	4.8
2	B	778	VAL	4.7
1	C	10	SER	4.7
1	C	30	GLU	4.6
2	B	385	GLY	4.6
1	C	34	LYS	4.5
2	B	783	GLU	4.5
1	C	44	THR	4.4
2	B	769	LEU	4.3
2	B	734	GLN	4.3
1	C	36	GLY	4.2
1	A	154	ASP	4.2
2	B	724	LEU	4.2
1	C	53	ARG	4.1
1	A	180	ALA	4.1
1	C	35	LYS	4.1
2	B	774	ILE	4.1
2	B	749	VAL	4.1
1	C	55	ALA	4.0
2	B	792	SER	4.0
1	C	27	VAL	4.0
2	D	732	VAL	4.0
2	B	391	VAL	3.9
2	B	202	THR	3.9
1	C	52	GLU	3.9
1	C	146	PRO	3.8
1	C	25	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	775	ALA	3.8
1	C	47	GLU	3.8
2	B	786	LYS	3.8
2	B	750	ALA	3.8
2	B	753	TYR	3.6
1	C	50	PRO	3.6
1	C	41	GLN	3.5
2	B	221	VAL	3.4
1	C	201	THR	3.4
1	C	24	LEU	3.2
1	C	56	ALA	3.2
1	C	15	ILE	3.2
2	B	203	LEU	3.2
1	C	6	GLU	3.2
2	B	198	THR	3.2
1	A	156	ASP	3.1
1	A	197	ASP	3.1
2	B	723	ILE	3.1
2	B	726	GLU	3.0
1	C	71	LEU	3.0
1	C	8	VAL	3.0
1	C	58	ALA	3.0
1	C	17	GLN	3.0
1	A	88	ALA	3.0
1	A	196	ASN	3.0
1	C	202	HIS	2.9
2	B	772	GLU	2.9
2	B	311	LEU	2.9
2	B	272	ILE	2.9
2	B	70	GLY	2.9
2	B	196	GLY	2.9
2	D	731	GLY	2.8
2	B	200	ASP	2.8
1	C	28	ARG	2.8
1	C	70	ALA	2.8
1	C	20	ASP	2.7
1	C	148	HIS	2.7
1	C	61	ASN	2.7
2	B	712	VAL	2.7
2	B	735	VAL	2.7
1	C	18	ALA	2.7
1	C	173	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	733	ASN	2.6
2	B	745	ARG	2.6
1	C	153	ALA	2.6
1	A	187	ILE	2.6
2	B	197	ALA	2.6
2	D	733	ASN	2.6
2	B	732	VAL	2.5
2	B	713	VAL	2.5
2	B	711	ALA	2.5
2	B	710	ILE	2.5
1	A	89	ALA	2.5
1	C	37	HIS	2.4
2	B	715	ALA	2.4
2	B	102	ASP	2.4
2	B	205	ILE	2.4
1	C	160	PHE	2.4
2	B	789	PHE	2.4
2	B	195	VAL	2.3
1	A	202	HIS	2.3
2	B	729	LYS	2.3
1	C	33	GLY	2.3
2	B	324	VAL	2.3
1	C	73	ALA	2.3
2	B	771	GLU	2.3
1	C	199	ASP	2.3
1	C	26	ASN	2.3
1	C	14	ALA	2.3
2	B	779	ALA	2.2
1	C	144	ASN	2.2
2	B	96	GLY	2.2
2	B	103	PHE	2.2
2	B	744	TYR	2.1
1	C	72	ASN	2.1
2	D	671	ARG	2.1
2	B	781	CYS	2.1
1	C	155	HIS	2.1
2	B	88	LEU	2.1
2	B	790	GLN	2.1
2	B	755	SER	2.1
1	C	250	PHE	2.1
2	B	776	ALA	2.1
2	B	207	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	749	VAL	2.1
2	B	703	PHE	2.1
1	A	148	HIS	2.1
2	B	761	ILE	2.0
2	B	204	PRO	2.0
1	C	68	GLN	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 monosaccharides 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
8	EDO	D	816	4/4	0.27	0.35	66,68,70,87	0
9	PGE	B	813	10/10	0.41	0.33	62,72,83,92	0
8	EDO	C	406	4/4	0.49	0.40	67,68,76,77	0
6	TRS	A	411	8/8	0.53	0.26	75,78,83,83	0
6	TRS	C	407	8/8	0.54	0.55	64,74,86,87	0
6	TRS	D	807	8/8	0.55	0.51	64,79,83,84	0
7	PEG	D	815	7/7	0.60	0.21	66,76,80,81	0
3	MG	D	801	1/1	0.61	0.14	74,74,74,74	0
4	CL	A	406	1/1	0.64	0.15	104,104,104,104	0
7	PEG	B	811	7/7	0.65	0.32	75,79,81,89	0
3	MG	D	802	1/1	0.66	0.42	91,91,91,91	0
7	PEG	B	812	7/7	0.67	0.27	66,68,77,86	0
8	EDO	B	807	4/4	0.70	0.21	61,66,71,75	0
8	EDO	D	818	4/4	0.71	0.13	71,71,71,83	0
7	PEG	B	810	7/7	0.71	0.29	60,68,75,75	0
7	PEG	B	809	7/7	0.73	0.21	54,63,76,78	0
8	EDO	D	812	4/4	0.74	0.35	72,73,75,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	PEG	C	404	7/7	0.75	0.17	51,64,78,81	0
9	PGE	B	806	10/10	0.75	0.25	57,65,73,84	0
7	PEG	A	409	7/7	0.75	0.27	67,76,80,88	0
6	TRS	A	408	8/8	0.76	0.25	50,62,67,68	0
8	EDO	C	408	4/4	0.76	0.20	60,61,64,69	0
8	EDO	B	814	4/4	0.77	0.25	53,63,67,67	0
5	HEZ	D	805	8/8	0.79	0.26	50,61,72,73	0
7	PEG	C	405	7/7	0.80	0.13	64,71,81,85	0
5	HEZ	D	803	8/8	0.81	0.21	57,62,68,76	0
3	MG	B	803	1/1	0.82	0.12	62,62,62,62	0
8	EDO	D	811	4/4	0.83	0.15	61,63,66,69	0
5	HEZ	D	806	8/8	0.83	0.22	45,50,55,59	0
8	EDO	B	815	4/4	0.84	0.17	65,70,73,79	0
7	PEG	D	813	7/7	0.84	0.14	40,55,61,65	0
5	HEZ	A	407	8/8	0.85	0.18	46,60,64,66	0
8	EDO	D	814	4/4	0.85	0.36	66,69,71,77	0
3	MG	A	404	1/1	0.86	0.23	68,68,68,68	0
5	HEZ	D	804	8/8	0.86	0.17	52,67,76,82	0
3	MG	B	801	1/1	0.88	0.24	69,69,69,69	0
8	EDO	D	808	4/4	0.88	0.22	54,54,62,71	0
3	MG	C	402	1/1	0.89	0.34	47,47,47,47	0
8	EDO	B	808	4/4	0.89	0.17	57,66,71,73	0
3	MG	B	804	1/1	0.89	0.26	78,78,78,78	0
3	MG	C	401	1/1	0.89	0.17	73,73,73,73	0
3	MG	A	403	1/1	0.90	0.16	56,56,56,56	0
3	MG	A	405	1/1	0.91	0.15	73,73,73,73	0
3	MG	A	401	1/1	0.92	0.29	48,48,48,48	0
8	EDO	D	817	4/4	0.92	0.12	60,65,65,75	0
8	EDO	C	403	4/4	0.93	0.20	50,51,69,84	0
7	PEG	B	805	7/7	0.93	0.13	60,64,71,73	0
8	EDO	D	809	4/4	0.93	0.16	48,49,49,52	0
8	EDO	D	810	4/4	0.94	0.14	61,61,64,71	0
3	MG	A	402	1/1	0.94	0.23	63,63,63,63	0
3	MG	B	802	1/1	0.98	0.14	58,58,58,58	0
8	EDO	A	410	4/4	0.98	0.14	54,61,63,64	0

6.5 Other polymers

There are no such residues in this entry.