Full wwPDB X-ray Structure Validation Report (i)

May 25, 2016 – 05:08 PM EDT

PDB ID	:	3PEF
Title	:	Crystal structure of gamma-hydroxybutyrate dehydrogenase from Geobacter metallireducens in complex with NADP+
Authors	:	Zhang, Y.; Garavito, R.M.
Deposited on	:	2010-10-26
Resolution	:	2.07 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:

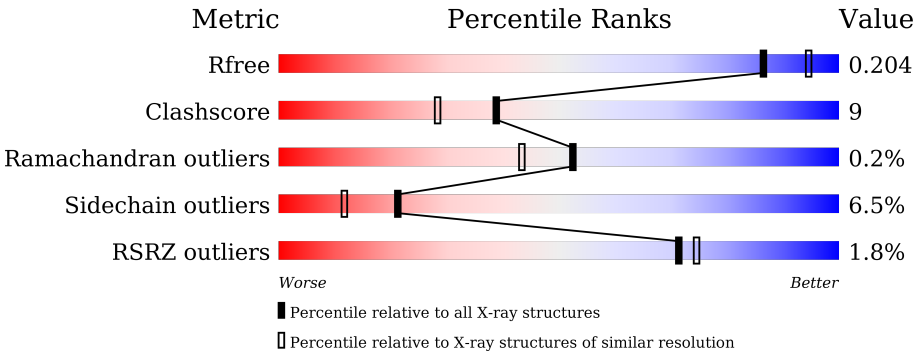
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027674
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027674

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 2.07 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	1799 (2.08-2.04)
Clashscore	102246	1910 (2.08-2.04)
Ramachandran outliers	100387	1893 (2.08-2.04)
Sidechain outliers	100360	1893 (2.08-2.04)
RSRZ outliers	91569	1802 (2.08-2.04)

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	287	85% 13% •
1	B	287	3% 82% 16% •
1	C	287	3% 82% 15% •
1	D	287	84% 15% •
1	E	287	87% 11% •
1	F	287	6% 78% 20% ••

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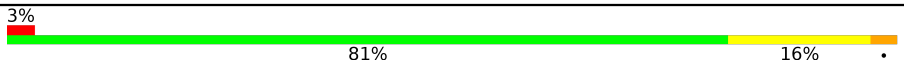
Mol	Chain	Length	Quality of chain
1	G	287	
1	H	287	

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	GOL	A	288	-	-	X	X
3	GOL	A	289	-	-	X	-
3	GOL	A	290	-	-	-	X
3	GOL	C	288	-	-	X	X
3	GOL	E	288	-	-	-	X
3	GOL	E	289	-	-	X	X
4	PEG	A	291	-	-	X	-
4	PEG	D	288	-	-	X	X
4	PEG	E	290	-	-	X	X
4	PEG	G	288	-	-	X	X
4	PEG	H	288	-	-	X	X
5	EDO	A	292	-	-	X	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 18166 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 6-phosphogluconate dehydrogenase, NAD-binding.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	1	0
			2095	1323	363	389	20			
1	B	287	Total	C	N	O	S	0	2	0
			2095	1324	360	389	22			
1	C	287	Total	C	N	O	S	0	0	0
			2087	1318	360	389	20			
1	D	286	Total	C	N	O	S	0	2	0
			2089	1320	359	390	20			
1	E	286	Total	C	N	O	S	0	2	0
			2092	1322	358	392	20			
1	F	285	Total	C	N	O	S	0	0	0
			2070	1309	355	386	20			
1	G	287	Total	C	N	O	S	0	0	0
			2087	1318	360	389	20			
1	H	286	Total	C	N	O	S	0	1	0
			2087	1319	359	389	20			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	MET	ENGINEERED MUTATION	UNP Q39R98
A	285	TYR	ILE	ENGINEERED MUTATION	UNP Q39R98
B	1	SER	MET	ENGINEERED MUTATION	UNP Q39R98
B	285	TYR	ILE	ENGINEERED MUTATION	UNP Q39R98
C	1	SER	MET	ENGINEERED MUTATION	UNP Q39R98
C	285	TYR	ILE	ENGINEERED MUTATION	UNP Q39R98
D	1	SER	MET	ENGINEERED MUTATION	UNP Q39R98
D	285	TYR	ILE	ENGINEERED MUTATION	UNP Q39R98
E	1	SER	MET	ENGINEERED MUTATION	UNP Q39R98
E	285	TYR	ILE	ENGINEERED MUTATION	UNP Q39R98
F	1	SER	MET	ENGINEERED MUTATION	UNP Q39R98
F	285	TYR	ILE	ENGINEERED MUTATION	UNP Q39R98
G	1	SER	MET	ENGINEERED MUTATION	UNP Q39R98

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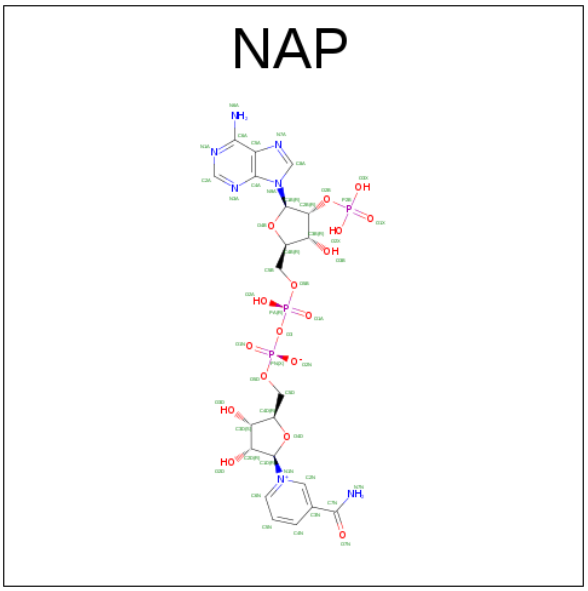
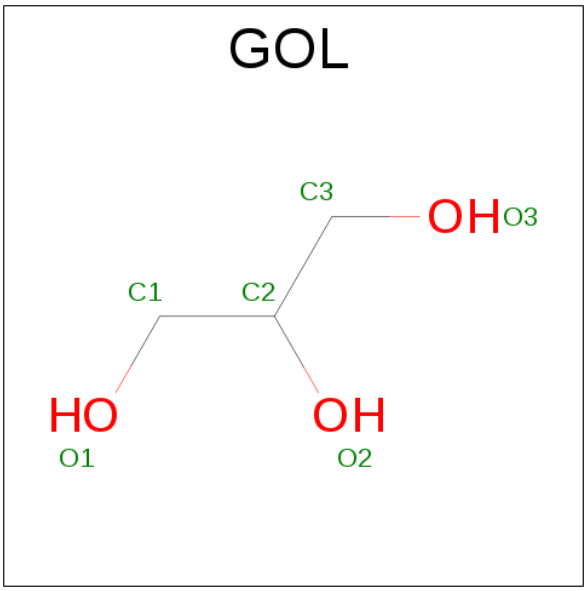
Chain	Residue	Modelled	Actual	Comment	Reference
G	285	TYR	ILE	ENGINEERED MUTATION	UNP Q39R98
H	1	SER	MET	ENGINEERED MUTATION	UNP Q39R98
H	285	TYR	ILE	ENGINEERED MUTATION	UNP Q39R98

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



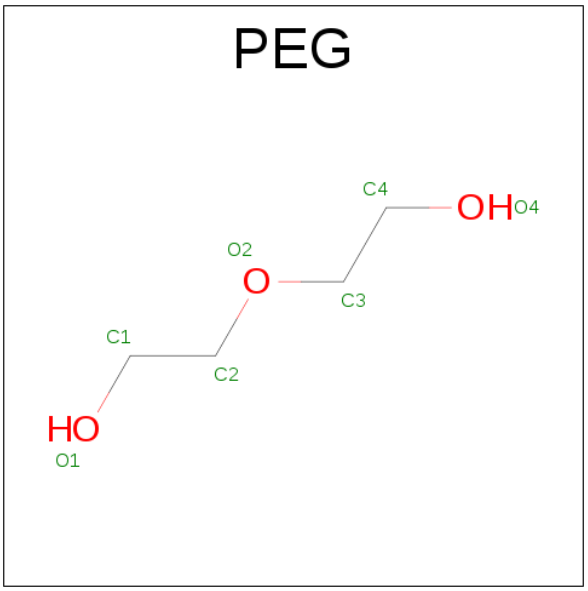
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



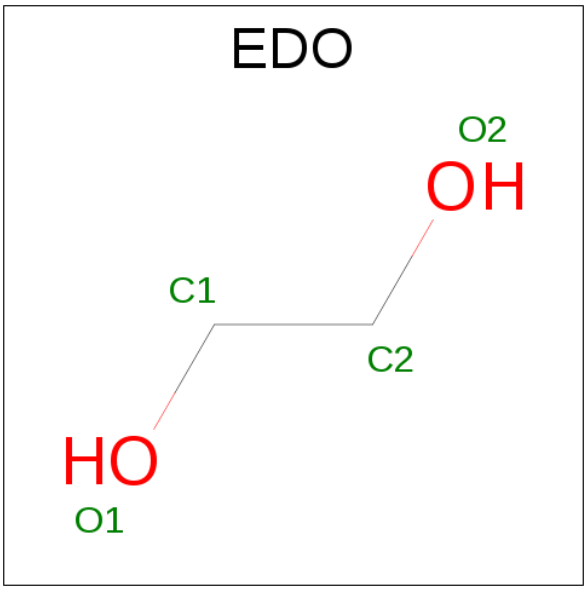
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0
3	E	1	Total C O 6 3 3	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	D	1	Total C O 7 4 3	0	0
4	E	1	Total C O 7 4 3	0	0
4	G	1	Total C O 7 4 3	0	0
4	H	1	Total C O 7 4 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 4 2 2	0	0

- Molecule 6 is water.

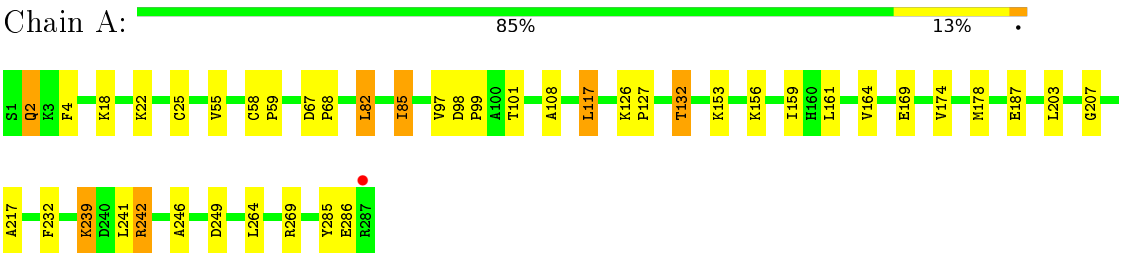
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	172	Total O 172 172	0	0
6	B	126	Total O 126 126	0	0
6	C	88	Total O 88 88	0	0
6	D	159	Total O 159 159	0	0
6	E	165	Total O 165 165	0	0
6	F	72	Total O 72 72	0	0
6	G	96	Total O 96 96	0	0
6	H	121	Total O 121 121	0	0

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.

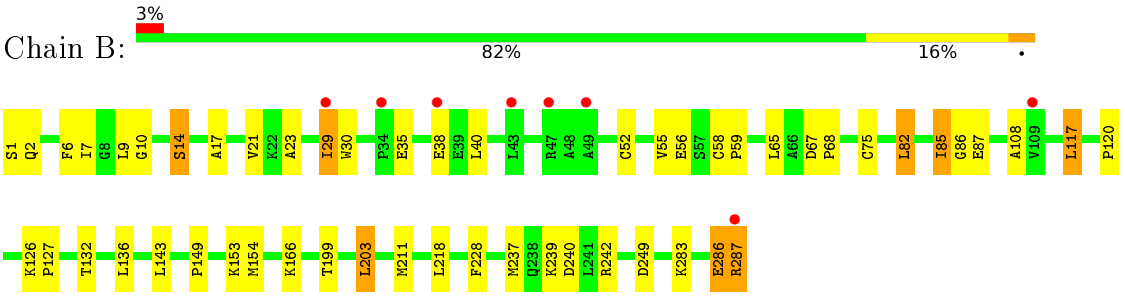
- Molecule 1: 6-phosphogluconate dehydrogenase, NAD-binding

Chain A:



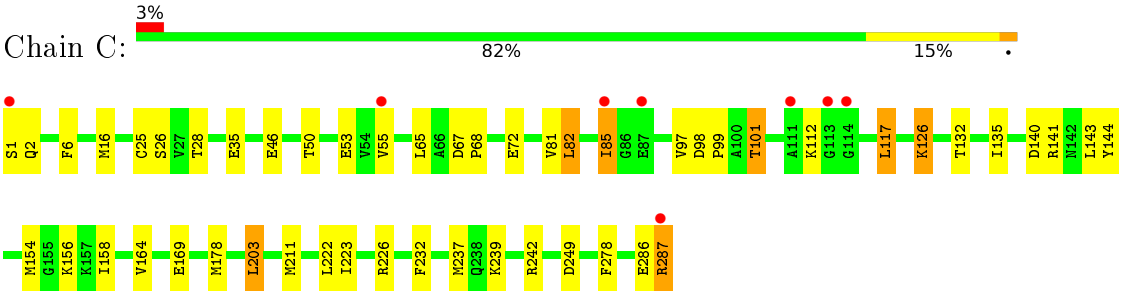
- Molecule 1: 6-phosphogluconate dehydrogenase, NAD-binding

Chain B:



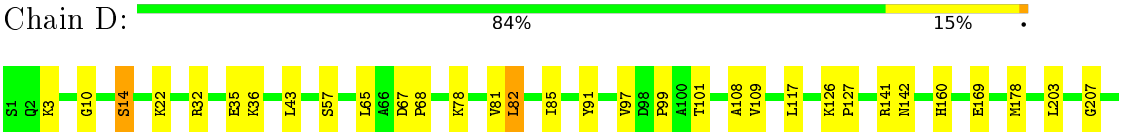
- Molecule 1: 6-phosphogluconate dehydrogenase, NAD-binding

Chain C:

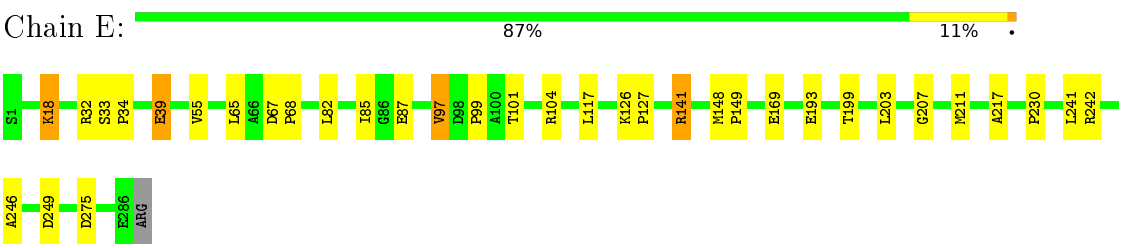


- Molecule 1: 6-phosphogluconate dehydrogenase, NAD-binding

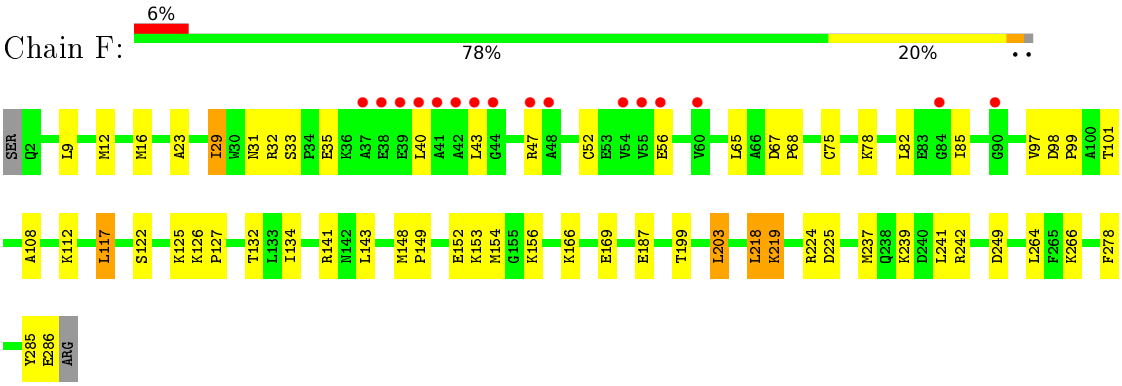
Chain D:



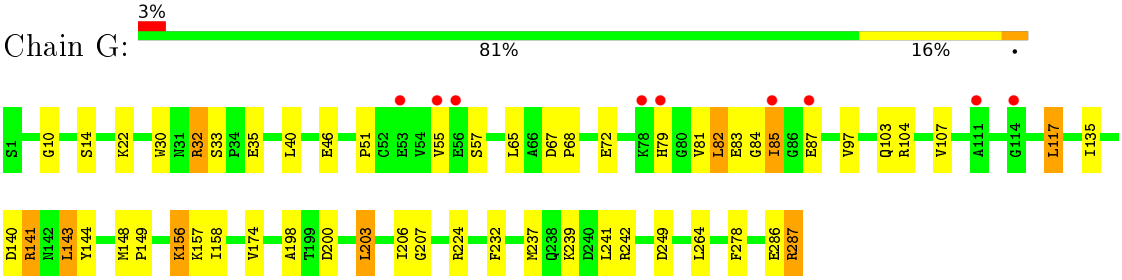
• Molecule 1: 6-phosphogluconate dehydrogenase, NAD-binding



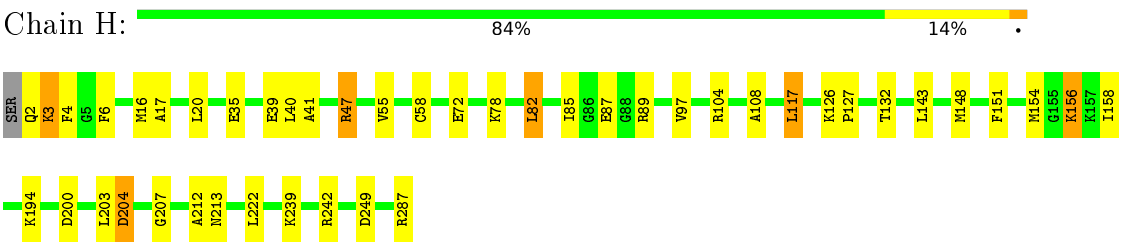
• Molecule 1: 6-phosphogluconate dehydrogenase, NAD-binding



• Molecule 1: 6-phosphogluconate dehydrogenase, NAD-binding



• Molecule 1: 6-phosphogluconate dehydrogenase, NAD-binding



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	75.97Å 79.14Å 95.47Å 82.15° 88.80° 87.66°	Depositor
Resolution (Å)	43.16 – 2.07 45.81 – 2.07	Depositor EDS
% Data completeness (in resolution range)	91.9 (43.16-2.07) 90.1 (45.81-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.93 (at 2.07Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.5_2)	Depositor
R, R_{free}	0.156 , 0.209 0.151 , 0.204	Depositor DCC
R_{free} test set	3745 reflections (3.04%)	DCC
Wilson B-factor (Å^2)	30.7	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 53.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.068 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	18166	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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: GOL, CSO, PEG, EDO, NAP

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	0.44	0/2123	0.61	3/2852 (0.1%)
1	B	0.43	0/2126	0.51	0/2856
1	C	0.44	0/2112	0.56	0/2838
1	D	0.38	0/2120	0.55	1/2849 (0.0%)
1	E	0.41	0/2117	0.56	0/2846
1	F	0.34	0/2095	0.49	0/2816
1	G	0.37	0/2112	0.54	0/2838
1	H	0.35	0/2115	0.53	1/2842 (0.0%)
All	All	0.40	0/16920	0.54	5/22737 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	222	LEU	O-C-N	-6.85	111.74	122.70
1	A	242	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	A	117	LEU	CA-CB-CG	6.21	129.59	115.30
1	A	242	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	D	222	LEU	O-C-N	-5.02	114.67	122.70

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	2095	0	2130	44	0
1	B	2095	0	2131	39	0
1	C	2087	0	2117	55	0
1	D	2089	0	2121	28	0
1	E	2092	0	2117	30	0
1	F	2070	0	2096	42	0
1	G	2087	0	2117	40	0
1	H	2087	0	2115	36	0
2	A	48	0	25	0	0
2	B	48	0	25	0	0
2	C	48	0	25	4	0
2	D	48	0	25	1	0
2	E	48	0	25	0	0
2	F	48	0	25	1	0
2	G	48	0	25	2	0
2	H	48	0	25	0	0
3	A	18	0	24	15	0
3	B	6	0	8	0	0
3	C	6	0	8	10	0
3	E	12	0	16	5	0
4	A	7	0	10	5	0
4	D	7	0	10	5	0
4	E	7	0	10	6	0
4	G	7	0	10	4	0
4	H	7	0	10	10	0
5	A	4	0	6	4	0
6	A	172	0	0	4	0
6	B	126	0	0	1	0
6	C	88	0	0	4	0
6	D	159	0	0	1	0
6	E	165	0	0	1	0
6	F	72	0	0	2	0
6	G	96	0	0	3	0
6	H	121	0	0	0	0
All	All	18166	0	17256	311	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 9.

All (311) 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:287:ARG:HH11	1:C:287:ARG:CG	1.64	1.11
1:C:287:ARG:HH11	1:C:287:ARG:HG3	1.17	1.09
1:A:269:ARG:HH12	3:A:289:GOL:H31	1.27	0.98
1:C:287:ARG:HB3	1:C:287:ARG:NH1	1.78	0.98
1:C:287:ARG:CB	1:C:287:ARG:NH1	2.30	0.94
1:H:212:ALA:HB1	4:H:288:PEG:H12	1.48	0.93
4:H:288:PEG:H41	4:H:288:PEG:H11	1.52	0.89
1:A:242:ARG:HH22	3:A:289:GOL:H32	1.35	0.88
1:B:132:THR:HG21	6:B:1035:HOH:O	1.74	0.88
1:D:217:ALA:HB2	4:D:288:PEG:H42	1.54	0.87
1:C:287:ARG:CG	1:C:287:ARG:NH1	2.34	0.85
1:H:213:ASN:H	4:H:288:PEG:H21	1.41	0.85
1:G:224:ARG:HG3	1:G:224:ARG:HH11	1.40	0.84
1:C:287:ARG:CZ	1:C:287:ARG:HB3	2.06	0.84
1:A:217:ALA:HB2	3:A:290:GOL:H11	1.60	0.83
1:A:242:ARG:HD3	1:D:249:ASP:OD1	1.79	0.82
1:A:246:ALA:HA	4:A:291:PEG:H12	1.62	0.81
1:C:287:ARG:HH11	1:C:287:ARG:CB	1.91	0.81
1:F:242:ARG:HD3	1:G:249:ASP:OD1	1.81	0.80
1:E:55[A]:VAL:HG21	1:E:85:ILE:HD12	1.64	0.79
1:D:217:ALA:HA	4:D:288:PEG:H11	1.65	0.79
1:F:249:ASP:OD1	1:G:242:ARG:HD3	1.85	0.77
1:C:178:MET:CE	3:C:288:GOL:H31	2.15	0.77
1:G:286:GLU:O	1:G:287:ARG:HB2	1.83	0.76
1:C:117:LEU:HB2	1:C:143:LEU:HD23	1.68	0.75
1:B:249:ASP:OD1	1:C:242:ARG:HD3	1.87	0.74
1:C:98:ASP:OD1	1:C:101:THR:HG23	1.87	0.74
1:B:242:ARG:HD3	1:C:249:ASP:OD1	1.86	0.74
1:A:269:ARG:NH1	3:A:289:GOL:H31	2.03	0.73
1:C:237:MET:HE2	1:C:278:PHE:CD2	2.23	0.72
1:F:97:VAL:CG1	1:F:101:THR:HB	2.19	0.72
1:A:82:LEU:HD21	1:A:108:ALA:HB1	1.72	0.72
1:A:249:ASP:OD1	1:D:242:ARG:HD3	1.89	0.71
1:E:217:ALA:HA	3:E:289:GOL:H2	1.72	0.71
1:H:151:PHE:HB3	1:H:158:ILE:HD13	1.72	0.71
1:G:82:LEU:HA	1:G:85:ILE:HD11	1.73	0.71
1:E:249:ASP:OD1	1:H:242:ARG:HD3	1.91	0.71
1:H:3:LYS:HE2	1:H:58:CYS:SG	2.32	0.70
1:A:207:GLY:HA3	3:A:290:GOL:H2	1.74	0.70
1:G:224:ARG:HG3	1:G:224:ARG:NH1	2.07	0.69
1:F:12:MET:HE1	1:F:125:LYS:HA	1.74	0.69
1:E:242:ARG:HD3	1:H:249:ASP:OD1	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:82:LEU:HD21	1:H:108:ALA:HB1	1.74	0.69
1:A:207:GLY:CA	3:A:290:GOL:H2	2.21	0.69
1:F:52:CSO:O	1:F:56:GLU:HG2	1.94	0.68
1:C:286:GLU:O	1:C:287:ARG:C	2.30	0.67
1:A:126:LYS:HB3	1:A:127:PRO:HD3	1.74	0.67
1:H:212:ALA:CB	4:H:288:PEG:H12	2.23	0.67
4:E:290:PEG:H11	1:H:242:ARG:HD2	1.76	0.67
1:A:127:PRO:HB3	1:A:132:THR:HG22	1.77	0.67
1:F:12:MET:HE2	1:F:12:MET:HA	1.77	0.66
1:G:232:PHE:HE1	1:G:237:MET:HE1	1.60	0.66
1:C:16:MET:HB3	1:C:154:MET:HE1	1.77	0.65
1:B:211:MET:SD	1:D:178:MET:HB2	2.36	0.65
1:E:97:VAL:HG13	1:E:101:THR:HB	1.79	0.65
1:C:286:GLU:OE2	1:C:287:ARG:NH2	2.30	0.65
1:E:207:GLY:HA2	3:E:289:GOL:H31	1.79	0.65
1:A:97:VAL:CG1	1:A:101:THR:HB	2.27	0.65
1:B:35:GLU:H	1:B:35:GLU:CD	1.99	0.64
1:G:232:PHE:CE1	1:G:237:MET:HE1	2.32	0.64
1:C:287:ARG:HG3	1:C:287:ARG:NH1	2.00	0.64
1:E:246:ALA:HB1	4:E:290:PEG:H21	1.80	0.64
1:F:16:MET:HB3	1:F:154:MET:HE1	1.80	0.64
1:D:213:ASN:H	4:D:288:PEG:H31	1.62	0.64
1:B:67:ASP:HB2	1:B:68:PRO:HD2	1.78	0.63
1:E:141:ARG:HG2	1:E:141:ARG:HH11	1.64	0.63
1:F:29:ILE:HD11	1:F:40:LEU:HD22	1.80	0.63
1:B:6:PHE:HE1	1:B:154[A]:MET:HE2	1.63	0.63
1:H:207:GLY:HA3	4:H:288:PEG:H41	1.81	0.63
1:E:39[A]:GLU:H	1:E:39[A]:GLU:CD	1.99	0.63
1:E:55[A]:VAL:CG2	1:E:85:ILE:HD12	2.29	0.62
1:A:97:VAL:HG13	1:A:101:THR:HB	1.82	0.62
1:A:99:PRO:HG3	1:A:169:GLU:HG3	1.81	0.62
1:A:269:ARG:HH12	3:A:289:GOL:C3	2.06	0.61
1:C:82:LEU:HD12	1:C:85:ILE:HD11	1.81	0.61
1:F:35:GLU:CD	1:F:35:GLU:H	2.05	0.61
1:H:126:LYS:HB3	1:H:127:PRO:HD3	1.82	0.61
1:A:232:PHE:CD1	3:A:288:GOL:H32	2.36	0.60
1:E:141:ARG:HH11	1:E:141:ARG:CG	2.14	0.60
1:G:67:ASP:HB2	1:G:68:PRO:HD2	1.84	0.60
1:B:67:ASP:HB3	1:B:239:LYS:HD3	1.82	0.60
1:G:206:ILE:HG22	4:G:288:PEG:H42	1.84	0.59
1:G:103:GLN:O	1:G:107:VAL:HG23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:VAL:O	1:C:85:ILE:HG13	2.03	0.59
1:C:67:ASP:HB2	1:C:68:PRO:HD2	1.83	0.58
2:C:301:NAP:C4N	3:C:288:GOL:H12	2.34	0.58
1:H:6:PHE:HE1	1:H:154:MET:HE2	1.69	0.58
1:G:237:MET:HE2	1:G:278:PHE:CD2	2.39	0.57
1:E:217:ALA:CA	3:E:289:GOL:H2	2.33	0.57
1:C:98:ASP:OD1	1:C:101:THR:CG2	2.52	0.56
1:C:203:LEU:HG	6:C:372:HOH:O	2.05	0.56
1:A:246:ALA:HB1	4:A:291:PEG:H32	1.88	0.56
1:G:81:VAL:O	1:G:85:ILE:HD13	2.06	0.56
1:B:228:PHE:CE2	1:B:283:LYS:HD2	2.41	0.56
1:A:242:ARG:NH2	3:A:289:GOL:H32	2.14	0.55
1:G:206:ILE:HG22	4:G:288:PEG:C4	2.36	0.55
1:G:237:MET:HE3	1:G:278:PHE:CE2	2.41	0.55
1:B:52:CSO:O	1:B:56:GLU:HB2	2.07	0.55
1:B:127:PRO:HB3	1:B:132:THR:HG23	1.88	0.55
1:E:246:ALA:CB	4:E:290:PEG:H21	2.36	0.55
6:F:668:HOH:O	1:G:242:ARG:HD2	2.06	0.55
1:G:117:LEU:HB2	1:G:143:LEU:HD13	1.89	0.54
1:H:6:PHE:CE1	1:H:154:MET:HE2	2.42	0.54
1:B:67:ASP:HB2	1:B:68:PRO:CD	2.36	0.54
1:D:97:VAL:HG13	1:D:101:THR:HB	1.88	0.54
1:F:67:ASP:HB2	1:F:68:PRO:HD2	1.90	0.54
1:B:7:ILE:HG23	1:B:30:TRP:CE3	2.42	0.54
1:F:12:MET:CE	1:F:125:LYS:HA	2.37	0.54
1:B:1:SER:HB2	1:H:287:ARG:HG3	1.88	0.54
1:F:16:MET:HB3	1:F:154:MET:CE	2.38	0.54
1:C:67:ASP:HB2	1:C:68:PRO:CD	2.37	0.54
1:A:55:VAL:HG11	1:A:85:ILE:HB	1.90	0.53
1:B:283:LYS:O	1:B:287:ARG:HB3	2.09	0.53
1:C:178:MET:HE3	3:C:288:GOL:H31	1.88	0.53
1:H:213:ASN:N	4:H:288:PEG:H21	2.18	0.53
1:E:246:ALA:HA	4:E:290:PEG:H12	1.90	0.53
1:G:237:MET:CE	1:G:278:PHE:CD2	2.91	0.53
1:A:249:ASP:HB3	4:A:291:PEG:H31	1.89	0.53
1:E:39[A]:GLU:N	1:E:39[A]:GLU:CD	2.62	0.53
1:C:55:VAL:HB	1:C:85:ILE:HG23	1.90	0.53
1:A:239:LYS:HB2	3:A:289:GOL:H2	1.91	0.53
1:C:178:MET:CE	1:C:237:MET:HE1	2.39	0.52
1:C:232:PHE:CE1	3:C:288:GOL:H11	2.44	0.52
1:B:9:LEU:HD11	1:B:29:ILE:HG23	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ASP:HB2	1:A:68:PRO:HD2	1.91	0.52
1:B:7:ILE:HG23	1:B:30:TRP:HE3	1.74	0.52
1:B:127:PRO:HA	1:B:132:THR:CG2	2.40	0.52
1:B:117:LEU:HB2	1:B:143:LEU:HD23	1.91	0.52
5:A:292:EDO:H12	6:A:701:HOH:O	2.08	0.52
1:C:223:ILE:O	1:C:226:ARG:HD3	2.09	0.52
1:E:104:ARG:HD3	6:E:651:HOH:O	2.10	0.52
1:F:218:LEU:HD13	1:F:219:LYS:HE2	1.91	0.52
1:G:224:ARG:CG	1:G:224:ARG:NH1	2.73	0.52
1:F:23:ALA:HB2	1:F:153:LYS:HD2	1.91	0.52
1:H:20:LEU:HG	1:H:154:MET:HE3	1.92	0.52
1:F:126:LYS:HB3	1:F:127:PRO:HD3	1.92	0.52
1:H:6:PHE:HE1	1:H:154:MET:CE	2.23	0.51
1:H:85:ILE:HA	1:H:89:ARG:HH12	1.75	0.51
4:A:291:PEG:H11	1:D:242:ARG:HD2	1.92	0.51
1:F:97:VAL:HG12	1:F:98:ASP:O	2.10	0.51
1:F:32:ARG:HB3	2:F:301:NAP:O1X	2.10	0.51
1:H:207:GLY:HA2	4:H:288:PEG:C1	2.41	0.51
1:A:242:ARG:HH22	3:A:289:GOL:C3	2.17	0.51
1:D:224:ARG:NH1	1:D:225:ASP:OD1	2.44	0.51
1:B:239:LYS:HE3	1:B:240:ASP:OD1	2.11	0.51
1:D:10:GLY:O	1:D:14:SER:HB2	2.10	0.51
1:H:207:GLY:CA	4:H:288:PEG:H41	2.41	0.50
1:G:135:ILE:HD12	1:G:158:ILE:HD12	1.92	0.50
1:A:264:LEU:HD13	1:A:285:TYR:OH	2.11	0.50
1:F:224:ARG:NH1	1:F:225:ASP:OD1	2.45	0.50
1:G:203:LEU:HG	6:G:839:HOH:O	2.11	0.50
1:A:242:ARG:HH12	3:A:289:GOL:C2	2.24	0.50
4:E:290:PEG:H11	1:H:242:ARG:CD	2.41	0.50
1:H:207:GLY:HA2	4:H:288:PEG:H12	1.93	0.50
2:C:301:NAP:C3N	3:C:288:GOL:H12	2.42	0.50
1:B:126:LYS:HB3	1:B:127:PRO:HD3	1.94	0.49
1:C:50:THR:OG1	1:C:53:GLU:HG3	2.11	0.49
1:D:67:ASP:HB2	1:D:68:PRO:HD2	1.94	0.49
1:C:82:LEU:O	1:C:112:LYS:HD3	2.12	0.49
1:H:132:THR:O	1:H:132:THR:HG22	2.12	0.49
1:B:38:GLU:HA	1:B:38:GLU:OE1	2.13	0.49
1:A:55:VAL:HG13	1:A:85:ILE:HD12	1.93	0.49
1:C:286:GLU:HB2	1:C:287:ARG:HE	1.77	0.49
1:E:99:PRO:HG3	1:E:169:GLU:HG3	1.94	0.49
1:F:97:VAL:CG1	1:F:98:ASP:N	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:ARG:NH1	1:E:141:ARG:CG	2.74	0.49
1:F:148:MET:HB3	1:F:149:PRO:HD3	1.94	0.49
1:C:126:LYS:HE2	6:C:335:HOH:O	2.13	0.48
1:G:141:ARG:O	1:G:144:TYR:HB3	2.12	0.48
1:A:132:THR:HG23	1:A:132:THR:O	2.12	0.48
1:B:82:LEU:HD21	1:B:108:ALA:HB1	1.94	0.48
1:D:99:PRO:HG3	1:D:169:GLU:HG3	1.93	0.48
1:C:232:PHE:CD1	3:C:288:GOL:H32	2.47	0.48
1:H:20:LEU:HD11	1:H:154:MET:HE1	1.95	0.48
1:A:132:THR:O	1:A:132:THR:CG2	2.62	0.48
1:A:178:MET:SD	3:A:288:GOL:H31	2.53	0.48
1:F:148:MET:O	1:F:152:GLU:HG3	2.13	0.48
1:A:159:ILE:HD12	1:A:161:LEU:HD21	1.95	0.48
1:C:135:ILE:HG13	1:C:158:ILE:HG12	1.96	0.48
1:F:132:THR:HG22	1:F:132:THR:O	2.14	0.48
1:F:29:ILE:CD1	1:F:40:LEU:HD22	2.42	0.48
1:G:32:ARG:HB3	2:G:301:NAP:O1X	2.14	0.48
1:B:10:GLY:O	1:B:14:SER:HB2	2.14	0.48
1:C:141:ARG:O	1:C:144:TYR:HB3	2.14	0.48
1:C:232:PHE:CD1	3:C:288:GOL:H11	2.49	0.48
1:G:72:GLU:OE2	1:G:104:ARG:NH2	2.47	0.48
1:G:55:VAL:HG11	1:G:81:VAL:HG13	1.96	0.48
1:H:132:THR:CG2	1:H:132:THR:O	2.61	0.48
4:H:288:PEG:H41	4:H:288:PEG:C1	2.32	0.48
1:A:242:ARG:CD	1:D:249:ASP:OD1	2.56	0.48
1:F:237:MET:HE3	1:F:278:PHE:CD2	2.48	0.48
1:D:3:LYS:HG3	6:D:319:HOH:O	2.14	0.47
1:G:10:GLY:O	1:G:14:SER:HB2	2.14	0.47
1:F:40:LEU:N	1:F:40:LEU:HD12	2.28	0.47
1:E:67:ASP:HB2	1:E:68:PRO:HD2	1.97	0.47
1:A:4:PHE:HE2	1:A:25:CYS:HG	1.62	0.47
1:B:86:GLY:C	1:B:87:GLU:HG2	2.34	0.47
1:D:207:GLY:HA2	4:D:288:PEG:H32	1.97	0.47
1:D:141:ARG:HD3	1:D:160:HIS:CE1	2.50	0.47
1:F:117:LEU:HB2	1:F:143:LEU:HD23	1.96	0.47
1:G:207:GLY:HA3	4:G:288:PEG:H12	1.98	0.46
1:A:232:PHE:CE1	3:A:288:GOL:H11	2.50	0.46
1:B:127:PRO:HA	1:B:132:THR:HG22	1.97	0.46
1:B:239:LYS:HB3	1:B:239:LYS:HE2	1.76	0.46
1:E:32:ARG:HG2	3:E:288:GOL:H2	1.96	0.46
1:A:178:MET:CE	3:A:288:GOL:H31	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:LYS:O	1:B:242:ARG:HB3	2.16	0.46
1:C:239:LYS:HB3	1:C:239:LYS:HE3	1.84	0.46
1:D:126:LYS:HB3	1:D:127:PRO:HD3	1.98	0.46
1:C:68:PRO:O	1:C:72:GLU:HG3	2.16	0.46
1:D:35:GLU:HB2	1:D:36:LYS:HE2	1.98	0.46
1:F:52:CSO:O	1:F:56:GLU:CG	2.63	0.46
1:B:120:PRO:HD2	1:B:136:LEU:O	2.15	0.46
1:D:85:ILE:HG12	1:D:109:VAL:HG13	1.97	0.46
1:E:211:MET:HE1	1:G:174:VAL:HG13	1.98	0.46
1:H:117:LEU:HB2	1:H:143:LEU:HD23	1.96	0.46
1:H:2:GLN:HG2	1:H:4:PHE:CE2	2.51	0.46
1:A:55:VAL:CG1	1:A:85:ILE:HD12	2.46	0.46
1:C:99:PRO:HG3	1:C:169:GLU:HG3	1.98	0.45
1:G:117:LEU:HB2	1:G:143:LEU:CD1	2.46	0.45
1:H:72:GLU:OE2	1:H:104:ARG:NH1	2.45	0.45
1:D:207:GLY:CA	4:D:288:PEG:H22	2.45	0.45
1:E:97:VAL:CG1	1:E:101:THR:HB	2.44	0.45
1:C:16:MET:HB3	1:C:154:MET:CE	2.45	0.45
1:F:23:ALA:CB	1:F:153:LYS:HD2	2.46	0.45
1:A:67:ASP:HB2	1:A:68:PRO:CD	2.47	0.45
2:C:301:NAP:C4N	3:C:288:GOL:C1	2.94	0.45
1:B:199:THR:HG22	1:B:203:LEU:HD22	1.98	0.45
1:A:174:VAL:HG13	1:C:211:MET:CE	2.47	0.45
1:C:164:VAL:HG23	6:C:706:HOH:O	2.16	0.45
1:E:18:LYS:HE2	1:E:39[B]:GLU:CD	2.37	0.44
1:H:16:MET:HB3	1:H:154:MET:HE2	1.99	0.44
1:E:217:ALA:CB	3:E:289:GOL:H2	2.47	0.44
1:E:126:LYS:HB3	1:E:127:PRO:HD3	2.00	0.44
1:A:187:GLU:HG3	1:A:285:TYR:CZ	2.52	0.44
1:C:178:MET:HE1	3:C:288:GOL:H31	1.99	0.44
1:C:211:MET:HG2	6:C:290:HOH:O	2.17	0.44
1:C:6:PHE:HE1	1:C:154:MET:CE	2.30	0.44
1:F:122:SER:HB3	1:F:134:ILE:HB	2.00	0.44
1:F:99:PRO:HG3	1:F:169:GLU:HG3	1.99	0.44
1:D:230:PRO:HG3	1:D:275:ASP:O	2.18	0.44
1:C:68:PRO:HB3	1:C:101:THR:HG21	2.00	0.44
1:C:98:ASP:CG	1:C:101:THR:HG23	2.36	0.44
1:E:67:ASP:HB2	1:E:68:PRO:CD	2.47	0.44
1:C:132:THR:HB	1:C:156:LYS:HD3	1.99	0.43
1:F:266:LYS:HE2	6:F:1024:HOH:O	2.17	0.43
1:B:17:ALA:O	1:B:21:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LYS:HE2	6:A:842:HOH:O	2.18	0.43
1:B:23:ALA:HB1	1:B:153:LYS:HE2	1.99	0.43
1:D:269[B]:ARG:NH1	1:D:274:GLY:HA3	2.34	0.43
1:G:148:MET:HB3	1:G:149:PRO:HD3	2.00	0.43
1:B:23:ALA:O	1:H:194:LYS:HE3	2.18	0.43
1:C:55:VAL:HG11	1:C:81:VAL:HG13	2.01	0.43
1:B:2:GLN:HE22	1:B:149:PRO:HG2	1.83	0.43
1:C:1:SER:O	1:C:25:CYS:HA	2.19	0.43
1:F:264:LEU:HD13	1:F:285:TYR:OH	2.18	0.43
4:A:291:PEG:H11	1:D:242:ARG:CD	2.49	0.43
1:C:85:ILE:HD12	1:C:112:LYS:HG2	2.00	0.43
1:G:55:VAL:HG23	1:G:84:GLY:HA3	2.01	0.43
1:H:41:ALA:HB2	1:H:47:ARG:HD3	1.99	0.43
1:B:58:CYS:HA	1:B:59:PRO:HD3	1.90	0.43
1:F:31:ASN:ND2	1:F:33:SER:H	2.16	0.42
1:F:67:ASP:HB2	1:F:68:PRO:CD	2.48	0.42
1:B:55:VAL:HB	1:B:85:ILE:HG12	2.01	0.42
2:C:301:NAP:H4N	3:C:288:GOL:H2	2.02	0.42
1:F:9:LEU:HD21	1:F:29:ILE:HG12	2.00	0.42
1:F:97:VAL:HG12	1:F:98:ASP:N	2.34	0.42
1:D:32:ARG:HB3	2:D:301:NAP:O1X	2.20	0.42
1:F:75:CYS:SG	1:F:82:LEU:HD13	2.60	0.42
4:G:288:PEG:H21	6:G:839:HOH:O	2.20	0.42
1:B:6:PHE:HE1	1:B:154[A]:MET:CE	2.32	0.42
1:F:166:LYS:HD3	1:F:166:LYS:HA	1.91	0.42
1:G:30:TRP:CE2	1:G:51:PRO:HD3	2.54	0.42
1:G:22:LYS:HE2	1:G:22:LYS:HB3	1.84	0.42
1:H:41:ALA:HB2	1:H:47:ARG:CD	2.49	0.42
1:H:151:PHE:HB3	1:H:158:ILE:CD1	2.46	0.42
1:H:156:LYS:H	1:H:156:LYS:HG3	1.65	0.42
1:A:164:VAL:HG21	5:A:292:EDO:H11	2.02	0.42
1:B:286:GLU:HB3	1:B:287:ARG:H	1.51	0.42
1:C:237:MET:CE	1:C:278:PHE:CD2	2.99	0.42
1:D:82:LEU:HD21	1:D:108:ALA:HB1	2.01	0.42
1:F:187:GLU:HG3	1:F:285:TYR:CZ	2.55	0.42
1:G:141:ARG:HE	1:G:141:ARG:HB3	1.49	0.42
1:F:97:VAL:HG11	1:F:101:THR:HB	2.01	0.41
1:G:79:HIS:N	1:G:83:GLU:OE2	2.53	0.41
1:A:132:THR:HG23	1:A:156:LYS:HE3	2.01	0.41
1:F:82:LEU:HD21	1:F:108:ALA:HB1	2.02	0.41
1:H:17:ALA:HB3	1:H:40:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:292:EDO:H21	6:A:662:HOH:O	2.21	0.41
1:A:97:VAL:CG1	1:A:98:ASP:N	2.83	0.41
1:F:199:THR:O	1:F:203:LEU:HD22	2.21	0.41
1:G:156:LYS:HG2	1:G:157:LYS:N	2.34	0.41
5:A:292:EDO:O2	6:A:293:HOH:O	2.12	0.41
1:E:246:ALA:HA	4:E:290:PEG:C1	2.51	0.41
1:C:178:MET:HE3	1:C:237:MET:HE1	2.01	0.41
2:G:301:NAP:H6N	6:G:457:HOH:O	2.21	0.41
1:A:58:CYS:HA	1:A:59:PRO:HD3	1.93	0.41
1:G:143:LEU:HD23	1:G:143:LEU:HA	1.89	0.41
1:G:33:SER:HB3	1:G:35:GLU:OE1	2.21	0.41
1:D:81:VAL:HG21	1:D:91:TYR:CZ	2.57	0.40
1:E:148:MET:N	1:E:149:PRO:CD	2.84	0.40
1:E:230:PRO:HG3	1:E:275:ASP:O	2.21	0.40
1:G:232:PHE:CE1	1:G:237:MET:CE	3.02	0.40
1:D:3:LYS:HE3	1:D:57:SER:O	2.21	0.40
1:E:33:SER:HA	1:E:34:PRO:HD3	1.85	0.40
1:H:200:ASP:O	1:H:204:ASP:HB2	2.21	0.40
1:C:28:THR:HA	1:C:46:GLU:HG2	2.03	0.40
1:B:75:CYS:SG	1:B:82:LEU:HD13	2.62	0.40
1:D:141:ARG:HA	1:D:141:ARG:HD2	1.74	0.40
1:C:82:LEU:HA	1:C:82:LEU:HD12	1.78	0.40
1:G:198:ALA:HB1	1:G:200:ASP:OD1	2.22	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	285/287 (99%)	277 (97%)	7 (2%)	1 (0%)	39	28
1	B	286/287 (100%)	277 (97%)	8 (3%)	1 (0%)	46	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	284/287 (99%)	274 (96%)	8 (3%)	2 (1%)	26 14
1	D	285/287 (99%)	278 (98%)	7 (2%)	0	100 100
1	E	285/287 (99%)	277 (97%)	8 (3%)	0	100 100
1	F	282/287 (98%)	272 (96%)	10 (4%)	0	100 100
1	G	284/287 (99%)	272 (96%)	11 (4%)	1 (0%)	39 28
1	H	284/287 (99%)	274 (96%)	10 (4%)	0	100 100
All	All	2275/2296 (99%)	2201 (97%)	69 (3%)	5 (0%)	52 43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	286	GLU
1	C	2	GLN
1	A	2	GLN
1	C	140	ASP
1	G	140	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	206/205 (100%)	195 (95%)	11 (5%)	28 18
1	B	207/205 (101%)	195 (94%)	12 (6%)	25 14
1	C	205/205 (100%)	193 (94%)	12 (6%)	24 14
1	D	206/205 (100%)	196 (95%)	10 (5%)	31 21
1	E	206/205 (100%)	193 (94%)	13 (6%)	22 12
1	F	203/205 (99%)	187 (92%)	16 (8%)	15 7
1	G	205/205 (100%)	187 (91%)	18 (9%)	12 5
1	H	205/205 (100%)	189 (92%)	16 (8%)	16 7
All	All	1643/1640 (100%)	1535 (93%)	108 (7%)	21 11

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	18	LYS
1	A	22	LYS
1	A	82	LEU
1	A	85	ILE
1	A	117	LEU
1	A	132	THR
1	A	203	LEU
1	A	239	LYS
1	A	241	LEU
1	A	286	GLU
1	B	14	SER
1	B	29	ILE
1	B	40	LEU
1	B	65	LEU
1	B	82	LEU
1	B	85	ILE
1	B	117	LEU
1	B	166	LYS
1	B	203	LEU
1	B	218	LEU
1	B	237	MET
1	B	287	ARG
1	C	26	SER
1	C	35	GLU
1	C	65	LEU
1	C	82	LEU
1	C	85	ILE
1	C	97	VAL
1	C	101	THR
1	C	117	LEU
1	C	126	LYS
1	C	203	LEU
1	C	222	LEU
1	C	287	ARG
1	D	14	SER
1	D	22	LYS
1	D	43	LEU
1	D	65	LEU
1	D	78	LYS
1	D	82	LEU
1	D	117	LEU

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Mol	Chain	Res	Type
1	D	142	ASN
1	D	203	LEU
1	D	239	LYS
1	E	18	LYS
1	E	39[A]	GLU
1	E	39[B]	GLU
1	E	65	LEU
1	E	82	LEU
1	E	87	GLU
1	E	97	VAL
1	E	117	LEU
1	E	141	ARG
1	E	193	GLU
1	E	199	THR
1	E	203	LEU
1	E	241	LEU
1	F	29	ILE
1	F	43	LEU
1	F	47	ARG
1	F	65	LEU
1	F	78	LYS
1	F	85	ILE
1	F	112	LYS
1	F	117	LEU
1	F	141	ARG
1	F	156	LYS
1	F	203	LEU
1	F	218	LEU
1	F	219	LYS
1	F	239	LYS
1	F	241	LEU
1	F	286	GLU
1	G	32	ARG
1	G	40	LEU
1	G	46	GLU
1	G	57	SER
1	G	65	LEU
1	G	82	LEU
1	G	85	ILE
1	G	87	GLU
1	G	97	VAL
1	G	117	LEU

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Mol	Chain	Res	Type
1	G	141	ARG
1	G	143	LEU
1	G	156	LYS
1	G	203	LEU
1	G	239	LYS
1	G	241	LEU
1	G	264	LEU
1	G	287	ARG
1	H	3	LYS
1	H	35	GLU
1	H	39[A]	GLU
1	H	39[B]	GLU
1	H	47	ARG
1	H	55	VAL
1	H	78	LYS
1	H	82	LEU
1	H	87	GLU
1	H	97	VAL
1	H	117	LEU
1	H	148	MET
1	H	156	LYS
1	H	203	LEU
1	H	204	ASP
1	H	239	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	B	2	GLN
1	F	2	GLN
1	G	79	HIS
1	G	142	ASN
1	H	79	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CSO	A	52	1	3,6,7	0.69	0	2,6,8	1.16	0
1	CSO	B	52	1	3,6,7	0.69	0	2,6,8	1.49	0
1	CSO	C	52	1	3,6,7	0.55	0	2,6,8	1.33	0
1	CSO	D	52	1	3,6,7	0.69	0	2,6,8	1.45	1 (50%)
1	CSO	E	52	1	3,6,7	1.01	0	2,6,8	1.30	0
1	CSO	F	52	1	3,6,7	0.51	0	2,6,8	1.51	1 (50%)
1	CSO	G	52	1	3,6,7	0.55	0	2,6,8	1.28	0
1	CSO	H	52	1	3,6,7	0.54	0	2,6,8	1.49	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
1	CSO	A	52	1	-	0/1/5/7	0/0/0/0
1	CSO	B	52	1	-	0/1/5/7	0/0/0/0
1	CSO	C	52	1	-	0/1/5/7	0/0/0/0
1	CSO	D	52	1	-	0/1/5/7	0/0/0/0
1	CSO	E	52	1	-	0/1/5/7	0/0/0/0
1	CSO	F	52	1	-	0/1/5/7	0/0/0/0
1	CSO	G	52	1	-	0/1/5/7	0/0/0/0
1	CSO	H	52	1	-	0/1/5/7	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	52	CSO	O-C-CA	-2.05	120.23	125.72
1	F	52	CSO	O-C-CA	-2.00	120.35	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	52	CSO	1	0
1	F	52	CSO	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

21 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	A	288	-	5,5,5	0.28	0	5,5,5	1.19	0
3	GOL	A	289	-	5,5,5	0.33	0	5,5,5	0.66	0
3	GOL	A	290	-	5,5,5	0.29	0	5,5,5	0.61	0
4	PEG	A	291	-	6,6,6	0.76	0	5,5,5	0.53	0
5	EDO	A	292	-	3,3,3	0.43	0	2,2,2	0.49	0
2	NAP	A	301	-	45,52,52	1.49	3 (6%)	55,80,80	1.92	6 (10%)
3	GOL	B	288	-	5,5,5	0.34	0	5,5,5	0.23	0
2	NAP	B	301	-	45,52,52	1.49	3 (6%)	55,80,80	1.83	5 (9%)
3	GOL	C	288	-	5,5,5	0.29	0	5,5,5	0.92	0
2	NAP	C	301	-	45,52,52	1.52	3 (6%)	55,80,80	1.97	6 (10%)
4	PEG	D	288	-	6,6,6	0.76	0	5,5,5	0.44	0
2	NAP	D	301	-	45,52,52	1.49	3 (6%)	55,80,80	2.01	7 (12%)
3	GOL	E	288	-	5,5,5	0.42	0	5,5,5	0.16	0
3	GOL	E	289	-	5,5,5	0.34	0	5,5,5	0.55	0
4	PEG	E	290	-	6,6,6	0.76	0	5,5,5	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAP	E	301	-	45,52,52	1.57	3 (6%)	55,80,80	1.84	6 (10%)
2	NAP	F	301	-	45,52,52	1.50	3 (6%)	55,80,80	1.82	4 (7%)
4	PEG	G	288	-	6,6,6	0.78	0	5,5,5	0.44	0
2	NAP	G	301	-	45,52,52	1.50	3 (6%)	55,80,80	1.82	5 (9%)
4	PEG	H	288	-	6,6,6	0.71	0	5,5,5	0.63	0
2	NAP	H	301	-	45,52,52	1.50	3 (6%)	55,80,80	1.98	5 (9%)

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	GOL	A	288	-	-	0/4/4/4	0/0/0/0
3	GOL	A	289	-	-	0/4/4/4	0/0/0/0
3	GOL	A	290	-	-	0/4/4/4	0/0/0/0
4	PEG	A	291	-	-	0/4/4/4	0/0/0/0
5	EDO	A	292	-	-	0/1/1/1	0/0/0/0
2	NAP	A	301	-	-	0/27/67/67	0/5/5/5
3	GOL	B	288	-	-	0/4/4/4	0/0/0/0
2	NAP	B	301	-	-	0/27/67/67	0/5/5/5
3	GOL	C	288	-	-	0/4/4/4	0/0/0/0
2	NAP	C	301	-	-	0/27/67/67	0/5/5/5
4	PEG	D	288	-	-	0/4/4/4	0/0/0/0
2	NAP	D	301	-	-	0/27/67/67	0/5/5/5
3	GOL	E	288	-	-	0/4/4/4	0/0/0/0
3	GOL	E	289	-	-	0/4/4/4	0/0/0/0
4	PEG	E	290	-	-	0/4/4/4	0/0/0/0
2	NAP	E	301	-	-	0/27/67/67	0/5/5/5
2	NAP	F	301	-	-	0/27/67/67	0/5/5/5
4	PEG	G	288	-	-	0/4/4/4	0/0/0/0
2	NAP	G	301	-	-	0/27/67/67	0/5/5/5
4	PEG	H	288	-	-	0/4/4/4	0/0/0/0
2	NAP	H	301	-	-	0/27/67/67	0/5/5/5

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	301	NAP	C2A-N1A	2.31	1.38	1.33
2	D	301	NAP	C2A-N1A	2.37	1.38	1.33
2	B	301	NAP	C2A-N1A	2.43	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	301	NAP	C2A-N1A	2.45	1.38	1.33
2	C	301	NAP	C2A-N1A	2.49	1.38	1.33
2	G	301	NAP	C2A-N1A	2.55	1.38	1.33
2	A	301	NAP	C2A-N1A	2.58	1.38	1.33
2	E	301	NAP	C2A-N1A	2.71	1.39	1.33
2	H	301	NAP	C2A-N3A	3.01	1.37	1.32
2	D	301	NAP	C2A-N3A	3.43	1.38	1.32
2	F	301	NAP	C2A-N3A	3.44	1.38	1.32
2	C	301	NAP	C2A-N3A	3.44	1.38	1.32
2	B	301	NAP	C2A-N3A	3.47	1.38	1.32
2	G	301	NAP	C2A-N3A	3.58	1.38	1.32
2	A	301	NAP	C2A-N3A	3.70	1.38	1.32
2	E	301	NAP	C2A-N3A	4.04	1.39	1.32
2	A	301	NAP	O7N-C7N	6.93	1.39	1.24
2	D	301	NAP	O7N-C7N	7.52	1.40	1.24
2	E	301	NAP	O7N-C7N	7.64	1.40	1.24
2	H	301	NAP	O7N-C7N	7.66	1.40	1.24
2	G	301	NAP	O7N-C7N	7.66	1.40	1.24
2	B	301	NAP	O7N-C7N	7.71	1.40	1.24
2	F	301	NAP	O7N-C7N	7.77	1.40	1.24
2	C	301	NAP	O7N-C7N	7.93	1.41	1.24

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	301	NAP	N3A-C2A-N1A	-12.06	119.40	128.87
2	H	301	NAP	N3A-C2A-N1A	-11.95	119.48	128.87
2	C	301	NAP	N3A-C2A-N1A	-11.70	119.68	128.87
2	B	301	NAP	N3A-C2A-N1A	-11.07	120.17	128.87
2	G	301	NAP	N3A-C2A-N1A	-11.07	120.17	128.87
2	A	301	NAP	N3A-C2A-N1A	-11.01	120.22	128.87
2	E	301	NAP	N3A-C2A-N1A	-10.94	120.28	128.87
2	F	301	NAP	N3A-C2A-N1A	-10.94	120.28	128.87
2	D	301	NAP	C1B-N9A-C4A	-3.46	122.94	126.81
2	D	301	NAP	O7N-C7N-C3N	-2.90	116.39	119.60
2	H	301	NAP	C1B-N9A-C4A	-2.78	123.70	126.81
2	C	301	NAP	C1B-N9A-C4A	-2.67	123.82	126.81
2	B	301	NAP	C1B-N9A-C4A	-2.61	123.90	126.81
2	A	301	NAP	O7N-C7N-C3N	-2.51	116.81	119.60
2	H	301	NAP	O7N-C7N-C3N	-2.40	116.93	119.60
2	E	301	NAP	O7N-C7N-N7N	-2.25	119.37	122.58
2	G	301	NAP	O7N-C7N-C3N	-2.20	117.16	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	301	NAP	C4B-O4B-C1B	-2.11	107.41	109.64
2	F	301	NAP	C1B-N9A-C4A	-2.08	124.49	126.81
2	E	301	NAP	C1B-N9A-C4A	-2.03	124.54	126.81
2	C	301	NAP	C3B-C2B-C1B	-2.01	98.77	102.63
2	E	301	NAP	C4D-O4D-C1D	2.03	111.80	109.64
2	G	301	NAP	O4B-C1B-N9A	2.06	111.99	108.11
2	G	301	NAP	O2X-P2B-O2B	2.10	112.91	106.62
2	D	301	NAP	C2N-C3N-C4N	2.19	120.75	118.27
2	E	301	NAP	O4B-C1B-N9A	2.20	112.27	108.11
2	A	301	NAP	O4B-C1B-N9A	2.21	112.28	108.11
2	F	301	NAP	C3N-C7N-N7N	2.22	120.33	117.82
2	D	301	NAP	O2N-PN-O1N	2.22	124.12	112.56
2	B	301	NAP	O2A-PA-O3	2.27	114.98	105.27
2	A	301	NAP	C4D-O4D-C1D	2.31	112.09	109.64
2	A	301	NAP	C2D-C1D-N1N	2.35	118.14	113.53
2	B	301	NAP	C3N-C7N-N7N	2.64	120.81	117.82
2	D	301	NAP	C3N-C7N-N7N	2.76	120.94	117.82
2	B	301	NAP	O4B-C1B-N9A	2.76	113.32	108.11
2	C	301	NAP	O4B-C1B-N9A	2.76	113.33	108.11
2	D	301	NAP	O4B-C1B-N9A	2.76	113.33	108.11
2	H	301	NAP	O4B-C1B-N9A	2.84	113.48	108.11
2	G	301	NAP	C3N-C7N-N7N	2.86	121.05	117.82
2	F	301	NAP	O4B-C1B-N9A	3.31	114.36	108.11
2	C	301	NAP	C3N-C7N-N7N	3.41	121.67	117.82
2	H	301	NAP	C3N-C7N-N7N	3.65	121.95	117.82
2	E	301	NAP	C3N-C7N-N7N	3.68	121.99	117.82
2	A	301	NAP	C3N-C7N-N7N	4.56	122.98	117.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 68 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	288	GOL	4	0
3	A	289	GOL	8	0
3	A	290	GOL	3	0
4	A	291	PEG	5	0
5	A	292	EDO	4	0
3	C	288	GOL	10	0
2	C	301	NAP	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	288	PEG	5	0
2	D	301	NAP	1	0
3	E	288	GOL	1	0
3	E	289	GOL	4	0
4	E	290	PEG	6	0
2	F	301	NAP	1	0
4	G	288	PEG	4	0
2	G	301	NAP	2	0
4	H	288	PEG	10	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	286/287 (99%)	-0.46	1 (0%) 94 95	18, 27, 45, 79	0
1	B	286/287 (99%)	-0.17	8 (2%) 56 62	22, 38, 64, 99	0
1	C	286/287 (99%)	-0.10	8 (2%) 56 62	20, 38, 69, 104	0
1	D	285/287 (99%)	-0.43	0 100 100	20, 31, 51, 80	0
1	E	285/287 (99%)	-0.48	0 100 100	19, 29, 45, 81	0
1	F	284/287 (98%)	0.10	16 (5%) 28 31	25, 45, 81, 111	0
1	G	286/287 (99%)	-0.02	9 (3%) 52 58	19, 40, 76, 101	0
1	H	285/287 (99%)	-0.18	0 100 100	21, 38, 60, 79	0
All	All	2283/2296 (99%)	-0.22	42 (1%) 71 74	18, 35, 67, 111	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	55	VAL	5.0
1	C	287	ARG	4.4
1	F	40	LEU	4.0
1	A	287	ARG	4.0
1	F	43	LEU	3.7
1	B	287	ARG	3.6
1	F	42	ALA	3.6
1	F	60	VAL	3.6
1	C	111	ALA	3.5
1	B	38	GLU	3.5
1	F	39	GLU	3.3
1	F	56	GLU	3.2
1	F	44	GLY	3.2
1	C	85	ILE	3.0
1	G	85	ILE	3.0
1	G	111	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	113	GLY	3.0
1	F	90	GLY	2.9
1	F	41	ALA	2.9
1	C	1	SER	2.8
1	C	55	VAL	2.8
1	G	114	GLY	2.8
1	B	47	ARG	2.7
1	F	37	ALA	2.7
1	G	56	GLU	2.6
1	F	47	ARG	2.6
1	F	84	GLY	2.5
1	G	78	LYS	2.4
1	F	48	ALA	2.4
1	B	49	ALA	2.4
1	F	38	GLU	2.3
1	G	87	GLU	2.3
1	B	109	VAL	2.2
1	G	53	GLU	2.2
1	B	29	ILE	2.2
1	C	87	GLU	2.1
1	C	114	GLY	2.1
1	B	34	PRO	2.1
1	F	54	VAL	2.1
1	G	79	HIS	2.0
1	B	43	LEU	2.0
1	G	55	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	CSO	H	52	7/8	0.91	0.17	-	47,52,64,89	0
1	CSO	B	52	7/8	0.92	0.17	-	41,46,70,87	0
1	CSO	D	52	7/8	0.96	0.07	-	32,35,53,72	0
1	CSO	E	52	7/8	0.96	0.10	-	25,29,42,81	0
1	CSO	G	52	7/8	0.89	0.14	-	61,63,89,102	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
1	CSO	A	52	7/8	0.92	0.10	-	22,26,45,73	0
1	CSO	C	52	7/8	0.94	0.18	-	51,55,67,87	0
1	CSO	F	52	7/8	0.89	0.18	-	65,67,74,103	0

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
5	EDO	A	292	4/4	0.93	0.36	13.39	44,48,48,49	0
4	PEG	G	288	7/7	0.85	0.27	13.01	30,36,51,58	0
3	GOL	A	288	6/6	0.75	0.25	12.13	43,47,53,53	0
4	PEG	H	288	7/7	0.74	0.19	9.56	46,55,67,70	0
3	GOL	C	288	6/6	0.85	0.20	5.78	41,51,56,57	0
4	PEG	D	288	7/7	0.85	0.14	5.48	29,44,49,51	0
3	GOL	E	288	6/6	0.81	0.17	5.15	51,55,61,64	0
3	GOL	E	289	6/6	0.90	0.14	3.98	24,39,46,47	0
4	PEG	E	290	7/7	0.84	0.28	3.64	31,52,66,68	0
3	GOL	A	290	6/6	0.87	0.15	2.69	26,43,52,55	0
4	PEG	A	291	7/7	0.86	0.20	1.69	35,51,60,66	0
3	GOL	A	289	6/6	0.90	0.13	0.52	36,41,48,57	0
2	NAP	A	301	48/48	0.99	0.09	-0.07	13,23,27,30	0
2	NAP	G	301	48/48	0.98	0.10	-0.20	24,39,56,56	0
2	NAP	B	301	48/48	0.97	0.09	-0.26	26,35,53,59	0
2	NAP	H	301	48/48	0.98	0.08	-0.37	22,31,37,41	0
2	NAP	F	301	48/48	0.97	0.10	-0.38	30,45,54,58	0
2	NAP	D	301	48/48	0.98	0.08	-0.44	15,26,33,35	0
2	NAP	C	301	48/48	0.98	0.08	-0.58	25,38,45,47	0
2	NAP	E	301	48/48	0.99	0.08	-0.71	17,24,29,32	0
3	GOL	B	288	6/6	0.85	0.18	-	74,75,78,79	0

6.5 Other polymers (i)

There are no such residues in this entry.