Full wwPDB X-ray Structure Validation Report (i)

Dec 3, 2023 – 09:41 am GMT

PDB ID	:	2C41
Title	:	X-ray structure of Dps from Thermosynechococcus elongatus
Authors	:	Ilari, A.; Franceschini, S.; Ceci, P.; Chiancone, E.
Deposited on	:	2005-10-14
Resolution	:	1.81 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

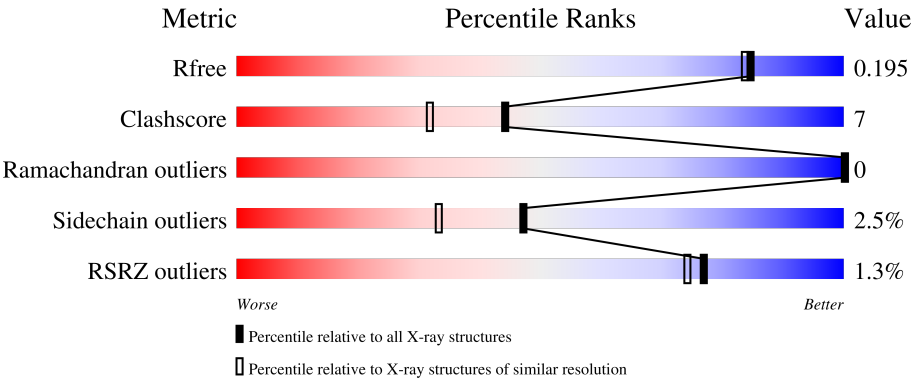
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.81 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	7484 (1.84-1.80)
Clashscore	141614	8401 (1.84-1.80)
Ramachandran outliers	138981	8290 (1.84-1.80)
Sidechain outliers	138945	8290 (1.84-1.80)
RSRZ outliers	127900	7371 (1.84-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	158	82% 16%
1	B	158	79% 18%
1	C	158	87% 13%
1	D	158	81% 16%
1	E	158	84% 13%

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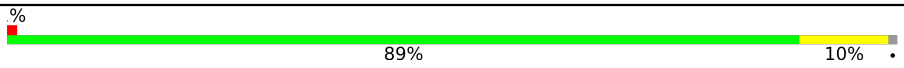
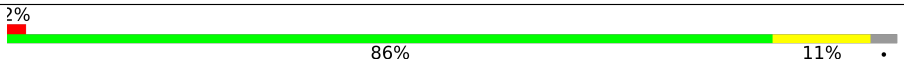
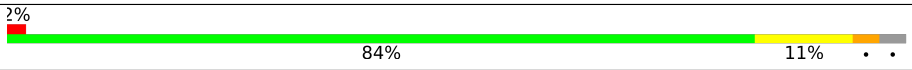
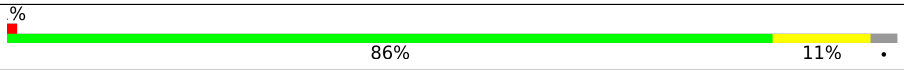
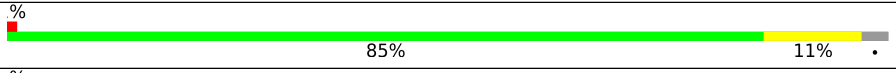
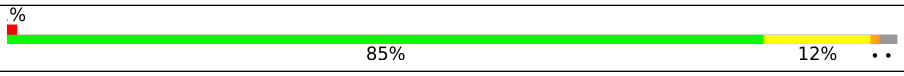
Mol	Chain	Length	Quality of chain
1	F	158	
1	G	158	
1	H	158	
1	I	158	
1	J	158	
1	K	158	
1	L	158	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16467 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 DPS FAMILY DNA-BINDING STRESS RESPONSE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	0	0	0
			1239	790	205	239	5			
1	B	154	Total	C	N	O	S	0	0	0
			1232	786	204	237	5			
1	C	157	Total	C	N	O	S	0	0	0
			1250	796	207	242	5			
1	D	154	Total	C	N	O	S	0	0	0
			1232	786	204	237	5			
1	E	154	Total	C	N	O	S	0	0	0
			1232	786	204	237	5			
1	F	156	Total	C	N	O	S	0	0	0
			1244	793	206	240	5			
1	G	154	Total	C	N	O	S	0	0	0
			1232	786	204	237	5			
1	H	154	Total	C	N	O	S	0	0	0
			1232	786	204	237	5			
1	I	154	Total	C	N	O	S	0	0	0
			1232	786	204	237	5			
1	J	153	Total	C	N	O	S	0	0	0
			1225	782	203	235	5			
1	K	153	Total	C	N	O	S	0	0	0
			1225	782	203	235	5			
1	L	155	Total	C	N	O	S	0	0	0
			1239	790	205	239	5			

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

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

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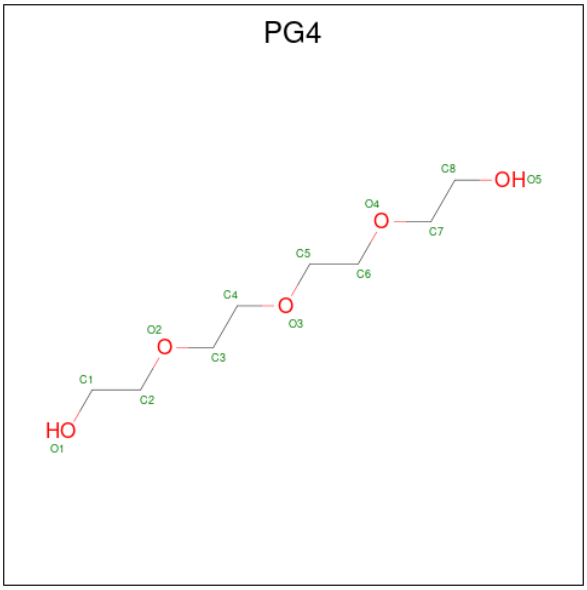
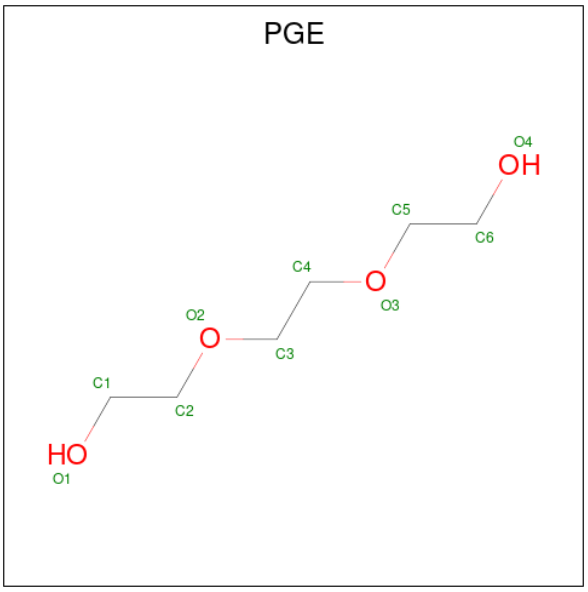
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total Cl 1 1	0	0
2	J	1	Total Cl 1 1	0	0

- Molecule 3 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 13 8 5	0	0
3	C	1	Total C O 13 8 5	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 10 6 4	0	0
4	B	1	Total C O 10 6 4	0	0
4	B	1	Total C O 10 6 4	0	0
4	C	1	Total C O 10 6 4	0	0
4	D	1	Total C O 10 6 4	0	0
4	E	1	Total C O 10 6 4	0	0
4	E	1	Total C O 10 6 4	0	0
4	F	1	Total C O 10 6 4	0	0
4	F	1	Total C O 10 6 4	0	0
4	H	1	Total C O 10 6 4	0	0
4	H	1	Total C O 10 6 4	0	0
4	L	1	Total C O 10 6 4	0	0

- Molecule 5 is water.

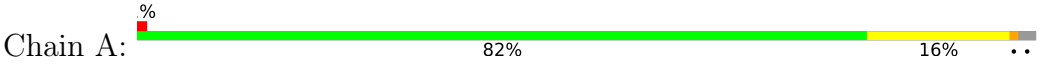
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	138	Total O 138 138	0	0
5	B	123	Total O 123 123	0	0
5	C	151	Total O 151 151	0	0
5	D	117	Total O 117 117	0	0
5	E	123	Total O 123 123	0	0
5	F	116	Total O 116 116	0	0
5	G	130	Total O 130 130	0	0
5	H	140	Total O 140 140	0	0
5	I	118	Total O 118 118	0	0
5	J	95	Total O 95 95	0	0
5	K	134	Total O 134 134	0	0
5	L	118	Total O 118 118	0	0

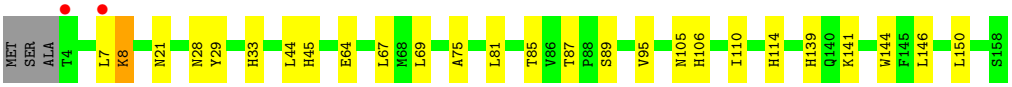
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DPS FAMILY DNA-BINDING STRESS RESPONSE PROTEIN

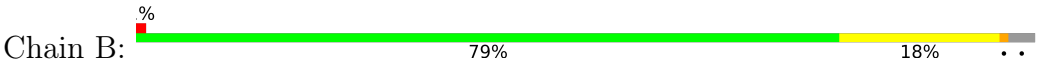
Chain A:

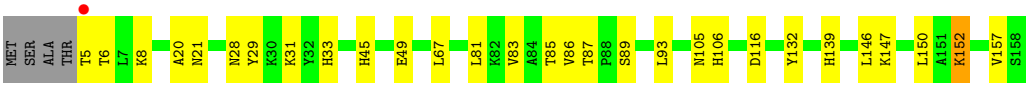




• Molecule 1: DPS FAMILY DNA-BINDING STRESS RESPONSE PROTEIN

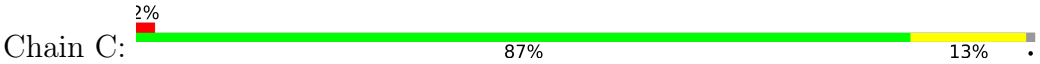
Chain B:

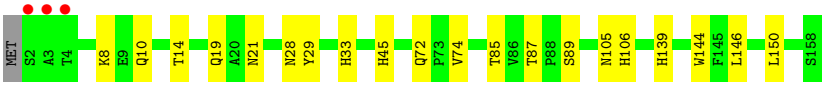




• Molecule 1: DPS FAMILY DNA-BINDING STRESS RESPONSE PROTEIN

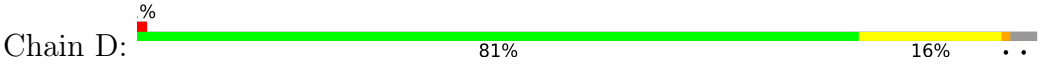
Chain C:

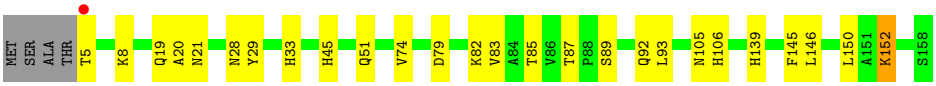




• Molecule 1: DPS FAMILY DNA-BINDING STRESS RESPONSE PROTEIN

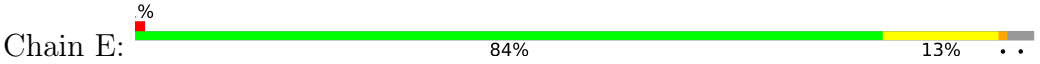
Chain D:

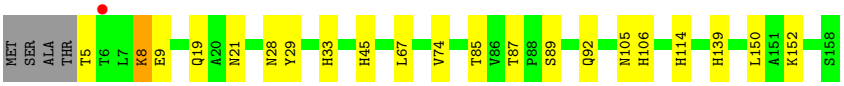




• Molecule 1: DPS FAMILY DNA-BINDING STRESS RESPONSE PROTEIN

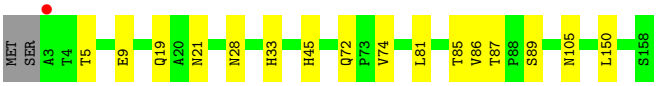
Chain E:





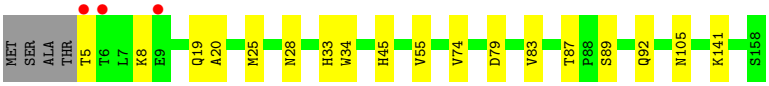
• Molecule 1: DPS FAMILY DNA-BINDING STRESS RESPONSE PROTEIN

Chain F:



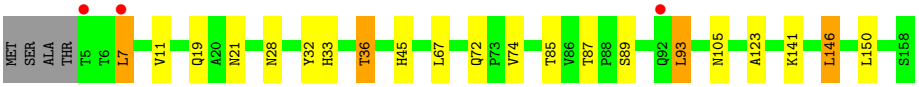
• Molecule 1: DPS FAMILY DNA-BINDING STRESS RESPONSE PROTEIN

Chain G:



• Molecule 1: DPS FAMILY DNA-BINDING STRESS RESPONSE PROTEIN

Chain H:

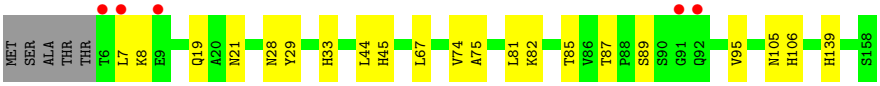


• Molecule 1: DPS FAMILY DNA-BINDING STRESS RESPONSE PROTEIN

Chain I:

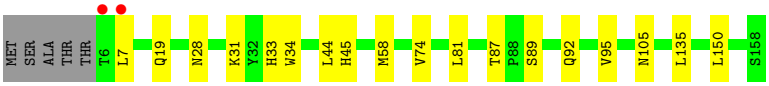
• Molecule 1: DPS FAMILY DNA-BINDING STRESS RESPONSE PROTEIN

Chain J:



• Molecule 1: DPS FAMILY DNA-BINDING STRESS RESPONSE PROTEIN

Chain K:



• Molecule 1: DPS FAMILY DNA-BINDING STRESS RESPONSE PROTEIN

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	122.97Å 122.89Å 253.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.81 29.88 – 1.81	Depositor EDS
% Data completeness (in resolution range)	97.3 (30.00-1.81) 97.2 (29.88-1.81)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.71 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.168 , 0.195 0.168 , 0.195	Depositor DCC
R_{free} test set	8507 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	18.6	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.025 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16467	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: CL, PGE, PG4

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	0.45	0/1263	0.56	0/1711
1	B	0.46	0/1256	0.56	0/1701
1	C	0.43	0/1274	0.53	0/1726
1	D	0.43	0/1256	0.53	0/1701
1	E	0.46	0/1256	0.51	0/1701
1	F	0.44	0/1268	0.50	0/1718
1	G	0.45	0/1256	0.51	0/1701
1	H	0.45	0/1256	0.55	2/1701 (0.1%)
1	I	0.44	0/1256	0.51	0/1701
1	J	0.45	0/1249	0.53	0/1691
1	K	0.45	0/1249	0.52	0/1691
1	L	0.45	0/1263	0.53	0/1711
All	All	0.45	0/15102	0.53	2/20454 (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	H	146	LEU	CA-CB-CG	5.35	127.60	115.30
1	H	93	LEU	CA-CB-CG	5.24	127.36	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	1239	0	1229	20	0
1	B	1232	0	1222	21	0
1	C	1250	0	1239	22	0
1	D	1232	0	1222	21	0
1	E	1232	0	1222	20	0
1	F	1244	0	1234	12	0
1	G	1232	0	1222	16	0
1	H	1232	0	1222	19	0
1	I	1232	0	1222	12	0
1	J	1225	0	1215	18	0
1	K	1225	0	1215	12	0
1	L	1239	0	1229	16	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	J	1	0	0	0	0
3	B	13	0	18	0	0
3	C	13	0	18	5	0
4	B	30	0	42	1	0
4	C	10	0	14	0	0
4	D	10	0	14	0	0
4	E	20	0	28	3	0
4	F	20	0	28	1	0
4	H	20	0	28	0	0
4	L	10	0	14	1	0
5	A	138	0	0	0	0
5	B	123	0	0	1	2
5	C	151	0	0	0	0
5	D	117	0	0	0	0
5	E	123	0	0	0	0
5	F	116	0	0	0	0
5	G	130	0	0	0	0
5	H	140	0	0	1	2
5	I	118	0	0	0	0
5	J	95	0	0	0	0
5	K	134	0	0	0	0
5	L	118	0	0	2	0
All	All	16467	0	14897	197	2

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 (197) 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:J:106:HIS:CD2	1:J:139:HIS:HD2	1.79	1.01
1:E:106:HIS:HD2	1:E:139:HIS:HD2	1.00	0.98
1:A:106:HIS:HD2	1:A:139:HIS:HD2	1.07	0.98
1:D:106:HIS:HD2	1:D:139:HIS:HD2	1.08	0.97
1:E:106:HIS:CD2	1:E:139:HIS:HD2	1.83	0.97
1:J:106:HIS:HD2	1:J:139:HIS:CD2	1.82	0.96
1:C:106:HIS:HD2	1:C:139:HIS:HD2	0.99	0.95
1:B:106:HIS:CD2	1:B:139:HIS:HD2	1.84	0.95
1:H:21:ASN:HD21	1:H:85:THR:H	1.15	0.93
1:B:106:HIS:HD2	1:B:139:HIS:HD2	1.03	0.93
1:D:21:ASN:HD21	1:D:85:THR:H	1.18	0.92
1:C:106:HIS:CD2	1:C:139:HIS:HD2	1.87	0.92
1:B:21:ASN:HD21	1:B:85:THR:H	1.18	0.89
1:J:21:ASN:HD21	1:J:85:THR:H	1.17	0.89
1:E:106:HIS:HD2	1:E:139:HIS:CD2	1.91	0.89
1:A:106:HIS:CD2	1:A:139:HIS:HD2	1.91	0.88
1:C:106:HIS:HD2	1:C:139:HIS:CD2	1.91	0.88
1:C:21:ASN:HD21	1:C:85:THR:H	1.18	0.88
1:J:106:HIS:HD2	1:J:139:HIS:HD2	0.94	0.87
1:D:106:HIS:CD2	1:D:139:HIS:HD2	1.92	0.86
1:B:106:HIS:HD2	1:B:139:HIS:CD2	1.92	0.86
1:A:21:ASN:HD21	1:A:85:THR:H	1.20	0.85
1:F:21:ASN:HD21	1:F:85:THR:H	1.23	0.84
1:A:106:HIS:HD2	1:A:139:HIS:CD2	1.96	0.82
1:L:21:ASN:HD21	1:L:85:THR:H	1.21	0.82
1:E:21:ASN:HD21	1:E:85:THR:H	1.24	0.82
1:D:106:HIS:HD2	1:D:139:HIS:CD2	1.98	0.81
1:I:21:ASN:HD21	1:I:85:THR:H	1.29	0.81
1:C:29:TYR:OH	1:C:106:HIS:HE1	1.65	0.80
1:A:29:TYR:OH	1:A:106:HIS:HE1	1.66	0.78
1:G:141:LYS:HD3	4:L:1159:PGE:H3	1.66	0.78
1:G:92:GLN:HE22	1:H:72:GLN:HE22	1.30	0.78
1:B:29:TYR:OH	1:B:106:HIS:HE1	1.70	0.75
1:E:29:TYR:OH	1:E:106:HIS:HE1	1.70	0.74
1:J:29:TYR:OH	1:J:106:HIS:HE1	1.70	0.73
1:B:28:ASN:HD21	1:B:89:SER:H	1.37	0.73
1:E:114:HIS:HB3	4:E:1159:PGE:H5	1.71	0.73
1:G:5:THR:HG22	1:G:8:LYS:HG3	1.71	0.72
1:H:87:THR:H	1:H:105:ASN:HD21	1.36	0.72
1:K:92:GLN:HE22	1:L:72:GLN:HE22	1.35	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:28:ASN:HD21	1:J:89:SER:H	1.36	0.72
1:B:87:THR:H	1:B:105:ASN:HD21	1.37	0.72
1:L:28:ASN:HD21	1:L:89:SER:H	1.38	0.72
1:A:28:ASN:HD21	1:A:89:SER:H	1.36	0.71
1:C:8:LYS:NZ	3:C:1159:PG4:H72	2.06	0.71
1:J:87:THR:H	1:J:105:ASN:HD21	1.37	0.71
1:F:28:ASN:HD21	1:F:89:SER:H	1.38	0.71
1:G:28:ASN:HD21	1:G:89:SER:H	1.39	0.70
1:H:28:ASN:HD21	1:H:89:SER:H	1.36	0.70
1:J:21:ASN:HD21	1:J:85:THR:N	1.89	0.70
1:D:20:ALA:CB	1:D:83:VAL:HG13	2.22	0.69
1:E:28:ASN:HD21	1:E:89:SER:H	1.39	0.69
1:D:29:TYR:OH	1:D:106:HIS:HE1	1.74	0.69
1:D:28:ASN:HD21	1:D:89:SER:H	1.39	0.68
1:K:87:THR:H	1:K:105:ASN:HD21	1.41	0.68
1:E:87:THR:H	1:E:105:ASN:HD21	1.42	0.68
1:I:28:ASN:HD21	1:I:89:SER:H	1.42	0.68
1:B:106:HIS:CD2	1:B:139:HIS:CD2	2.75	0.67
1:C:28:ASN:HD21	1:C:89:SER:H	1.40	0.67
1:E:106:HIS:CD2	1:E:139:HIS:CD2	2.75	0.66
1:C:21:ASN:HD21	1:C:85:THR:N	1.93	0.66
1:C:87:THR:H	1:C:105:ASN:HD21	1.44	0.66
1:A:21:ASN:HD21	1:A:85:THR:N	1.92	0.65
1:J:106:HIS:CD2	1:J:139:HIS:CD2	2.68	0.65
1:L:21:ASN:HD21	1:L:85:THR:N	1.94	0.65
1:L:122:GLU:OE2	5:L:2092:HOH:O	2.14	0.65
1:C:8:LYS:HE2	3:C:1159:PG4:H21	1.77	0.65
1:F:21:ASN:HD21	1:F:85:THR:N	1.95	0.65
1:F:87:THR:H	1:F:105:ASN:HD21	1.45	0.65
1:L:87:THR:H	1:L:105:ASN:HD21	1.44	0.64
1:A:87:THR:H	1:A:105:ASN:HD21	1.45	0.64
1:A:8:LYS:HD3	1:A:69:LEU:O	1.98	0.64
1:C:72:GLN:HE22	1:D:92:GLN:HE22	1.47	0.63
1:I:87:THR:H	1:I:105:ASN:HD21	1.44	0.63
1:J:19:GLN:HE22	1:J:74:VAL:H	1.47	0.62
1:H:32:TYR:O	1:H:36:THR:OG1	2.17	0.62
1:K:31:LYS:HG3	1:L:75:ALA:HB1	1.80	0.62
1:D:21:ASN:HD21	1:D:85:THR:N	1.93	0.61
1:K:28:ASN:HD21	1:K:89:SER:H	1.48	0.61
1:B:21:ASN:HD21	1:B:85:THR:N	1.94	0.60
1:A:141:LYS:HD3	4:E:1160:PGE:H3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:HIS:HB3	4:E:1159:PGE:C5	2.32	0.59
1:I:5:THR:HB	1:I:9:GLU:HG3	1.85	0.59
1:A:28:ASN:ND2	1:A:89:SER:H	2.01	0.58
1:H:21:ASN:HD21	1:H:85:THR:N	1.93	0.58
1:J:28:ASN:ND2	1:J:89:SER:H	2.01	0.58
1:G:87:THR:H	1:G:105:ASN:HD21	1.52	0.58
1:L:28:ASN:ND2	1:L:89:SER:H	2.02	0.58
1:G:20:ALA:CB	1:G:83:VAL:HG13	2.33	0.58
1:C:106:HIS:CD2	1:C:139:HIS:CD2	2.78	0.57
1:H:28:ASN:ND2	1:H:89:SER:H	2.01	0.57
1:C:8:LYS:HE3	3:C:1159:PG4:H61	1.86	0.57
1:K:19:GLN:HE22	1:K:74:VAL:H	1.52	0.57
1:L:7:LEU:HG	1:L:123:ALA:HB2	1.86	0.57
1:D:20:ALA:HB2	1:D:83:VAL:HG13	1.87	0.57
1:E:92:GLN:HE22	1:F:72:GLN:HE22	1.50	0.57
1:H:19:GLN:HE22	1:H:74:VAL:H	1.53	0.57
1:D:5:THR:HG22	1:D:8:LYS:HG3	1.87	0.56
1:D:28:ASN:ND2	1:D:89:SER:H	2.04	0.56
1:F:28:ASN:ND2	1:F:89:SER:H	2.03	0.56
1:E:28:ASN:ND2	1:E:89:SER:H	2.02	0.55
1:D:33:HIS:CE1	1:D:45:HIS:CE1	2.94	0.55
1:G:79:ASP:O	1:G:83:VAL:HG12	2.07	0.55
1:I:28:ASN:ND2	1:I:89:SER:H	2.03	0.55
1:E:21:ASN:HD21	1:E:85:THR:N	1.98	0.54
1:J:19:GLN:HE22	1:J:74:VAL:N	2.05	0.54
1:C:28:ASN:ND2	1:C:89:SER:H	2.05	0.54
1:G:28:ASN:ND2	1:G:89:SER:H	2.05	0.53
1:H:7:LEU:H	1:H:7:LEU:CD2	2.21	0.53
1:I:21:ASN:HD21	1:I:85:THR:N	2.00	0.53
1:C:8:LYS:HZ1	3:C:1159:PG4:H72	1.73	0.53
1:B:28:ASN:ND2	1:B:89:SER:H	2.05	0.52
1:C:19:GLN:HE22	1:C:74:VAL:H	1.56	0.52
1:D:106:HIS:CD2	1:D:139:HIS:CD2	2.83	0.52
1:G:20:ALA:HB2	1:G:83:VAL:HG13	1.93	0.51
1:L:81:LEU:HD23	5:L:2052:HOH:O	2.10	0.51
1:H:36:THR:HG22	5:H:2034:HOH:O	2.11	0.51
1:B:147:LYS:HG2	4:B:1160:PGE:H4	1.93	0.51
1:G:19:GLN:HE22	1:G:74:VAL:H	1.58	0.50
1:A:110:ILE:O	1:A:114:HIS:HD2	1.95	0.50
1:A:44:LEU:HD13	1:A:95:VAL:HG11	1.94	0.50
1:E:19:GLN:HE22	1:E:74:VAL:H	1.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:THR:HG23	1:B:8:LYS:H	1.77	0.49
1:J:67:LEU:HD13	1:L:144:TRP:CZ2	2.47	0.49
1:G:5:THR:HG23	1:G:8:LYS:H	1.78	0.49
1:A:144:TRP:CZ2	1:E:67:LEU:HD13	2.47	0.49
1:K:19:GLN:HE22	1:K:74:VAL:N	2.10	0.49
1:A:106:HIS:CD2	1:A:139:HIS:CD2	2.82	0.49
1:C:33:HIS:CE1	1:C:45:HIS:CE1	3.01	0.48
1:F:33:HIS:CE1	1:F:45:HIS:CE1	3.01	0.48
1:E:33:HIS:CE1	1:E:45:HIS:CE1	3.01	0.48
1:D:19:GLN:HE22	1:D:74:VAL:H	1.62	0.48
1:F:19:GLN:HE22	1:F:74:VAL:H	1.61	0.48
1:I:33:HIS:CE1	1:I:45:HIS:CE1	3.02	0.47
1:H:19:GLN:HE22	1:H:74:VAL:N	2.10	0.47
1:J:87:THR:H	1:J:105:ASN:ND2	2.11	0.47
1:K:33:HIS:CE1	1:K:45:HIS:CE1	3.03	0.47
1:H:7:LEU:H	1:H:7:LEU:HD22	1.79	0.47
1:C:8:LYS:HZ2	3:C:1159:PG4:H72	1.79	0.47
1:D:87:THR:H	1:D:105:ASN:HD21	1.61	0.47
1:L:33:HIS:CE1	1:L:45:HIS:CE1	3.04	0.46
1:K:28:ASN:ND2	1:K:89:SER:H	2.11	0.46
1:I:19:GLN:HE22	1:I:74:VAL:H	1.63	0.46
1:J:44:LEU:HD13	1:J:95:VAL:HG11	1.97	0.46
1:F:21:ASN:ND2	1:F:86:VAL:H	2.14	0.46
1:G:19:GLN:HE22	1:G:74:VAL:N	2.14	0.46
1:C:19:GLN:HE22	1:C:74:VAL:N	2.13	0.46
1:E:87:THR:H	1:E:105:ASN:ND2	2.12	0.45
1:A:29:TYR:OH	1:A:106:HIS:CE1	2.57	0.45
1:L:44:LEU:HD13	1:L:95:VAL:HG11	1.98	0.45
1:D:152:LYS:HB3	1:D:152:LYS:HE3	1.54	0.44
1:H:7:LEU:O	1:H:11:VAL:HG23	2.16	0.44
1:B:157:VAL:HA	5:B:2116:HOH:O	2.17	0.44
1:J:33:HIS:CE1	1:J:45:HIS:CE1	3.06	0.44
1:H:33:HIS:CE1	1:H:45:HIS:CE1	3.04	0.44
1:L:87:THR:H	1:L:105:ASN:ND2	2.13	0.44
1:G:33:HIS:CE1	1:G:45:HIS:CE1	3.05	0.44
1:H:7:LEU:HG	1:H:123:ALA:HA	1.99	0.44
1:F:19:GLN:HE22	1:F:74:VAL:N	2.16	0.44
1:K:87:THR:H	1:K:105:ASN:ND2	2.12	0.43
1:F:5:THR:O	1:F:9:GLU:HG2	2.17	0.43
1:K:58:MET:HG2	1:K:135:LEU:HD22	2.01	0.43
1:C:10:GLN:O	1:C:14:THR:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:34:TRP:HB3	1:L:67:LEU:HD21	2.01	0.43
1:I:19:GLN:HE22	1:I:74:VAL:N	2.17	0.42
1:B:20:ALA:HB2	1:B:83:VAL:HG23	2.00	0.42
1:B:116:ASP:HB3	1:B:132:TYR:CE1	2.54	0.42
1:C:144:TRP:CZ2	1:H:67:LEU:HD13	2.54	0.42
1:E:5:THR:OG1	1:E:8:LYS:HB2	2.19	0.42
1:E:19:GLN:HE22	1:E:74:VAL:N	2.17	0.42
1:I:31:LYS:HG3	1:J:75:ALA:HB1	2.01	0.42
1:A:64:GLU:HA	1:A:67:LEU:HD23	2.02	0.42
1:B:20:ALA:CB	1:B:83:VAL:HG23	2.49	0.42
1:I:6:THR:OG1	1:I:9:GLU:HG2	2.20	0.42
1:B:33:HIS:CE1	1:B:45:HIS:CE1	3.08	0.42
1:C:29:TYR:OH	1:C:106:HIS:CE1	2.57	0.41
1:H:105:ASN:HD22	1:H:105:ASN:HA	1.73	0.41
1:A:33:HIS:CE1	1:A:45:HIS:CE1	3.08	0.41
1:B:33:HIS:CE1	1:B:49:GLU:HB2	2.56	0.41
1:D:19:GLN:HE22	1:D:74:VAL:N	2.19	0.41
1:B:21:ASN:ND2	1:B:86:VAL:H	2.19	0.41
1:D:51:GLN:HE22	1:D:145:PHE:HB2	1.86	0.41
1:D:105:ASN:HD22	1:D:105:ASN:HA	1.68	0.41
1:E:9:GLU:H	1:E:9:GLU:HG2	1.76	0.41
4:F:1160:PGE:H3	1:H:141:LYS:HD3	2.02	0.41
1:A:8:LYS:HE3	1:A:69:LEU:HB3	2.03	0.41
1:J:7:LEU:HD23	1:J:8:LYS:HD3	2.02	0.41
1:D:79:ASP:O	1:D:83:VAL:HG12	2.21	0.41
1:G:25:MET:HB3	1:G:55:VAL:HG11	2.03	0.41
1:G:34:TRP:HB3	1:H:67:LEU:HD11	2.03	0.41
1:B:152:LYS:HB3	1:B:152:LYS:HE3	1.73	0.40
1:G:87:THR:H	1:G:105:ASN:ND2	2.18	0.40
1:I:18:GLU:HG3	1:I:132:TYR:CE2	2.56	0.40
1:L:19:GLN:HE22	1:L:74:VAL:H	1.67	0.40
1:A:75:ALA:HB1	1:B:31:LYS:HG3	2.03	0.40
1:F:21:ASN:ND2	1:F:85:THR:H	2.05	0.40
1:K:44:LEU:HD13	1:K:95:VAL:HG11	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:2067:HOH:O	5:H:2072:HOH:O[5_445]	2.06	0.14
5:B:2067:HOH:O	5:H:2067:HOH:O[5_445]	2.13	0.07

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	153/158 (97%)	151 (99%)	2 (1%)	0	100	100
1	B	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
1	C	155/158 (98%)	153 (99%)	2 (1%)	0	100	100
1	D	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
1	E	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
1	F	154/158 (98%)	152 (99%)	2 (1%)	0	100	100
1	G	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
1	H	152/158 (96%)	151 (99%)	1 (1%)	0	100	100
1	I	152/158 (96%)	150 (99%)	2 (1%)	0	100	100
1	J	151/158 (96%)	149 (99%)	2 (1%)	0	100	100
1	K	151/158 (96%)	149 (99%)	2 (1%)	0	100	100
1	L	153/158 (97%)	151 (99%)	2 (1%)	0	100	100
All	All	1829/1896 (96%)	1806 (99%)	23 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	133/135 (98%)	128 (96%)	5 (4%)	33	18
1	B	132/135 (98%)	125 (95%)	7 (5%)	22	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	134/135 (99%)	132 (98%)	2 (2%)	65	55
1	D	132/135 (98%)	127 (96%)	5 (4%)	33	18
1	E	132/135 (98%)	129 (98%)	3 (2%)	50	37
1	F	133/135 (98%)	131 (98%)	2 (2%)	65	55
1	G	132/135 (98%)	132 (100%)	0	100	100
1	H	132/135 (98%)	127 (96%)	5 (4%)	33	18
1	I	132/135 (98%)	130 (98%)	2 (2%)	65	55
1	J	131/135 (97%)	129 (98%)	2 (2%)	65	55
1	K	131/135 (97%)	128 (98%)	3 (2%)	50	37
1	L	133/135 (98%)	130 (98%)	3 (2%)	50	37
All	All	1587/1620 (98%)	1548 (98%)	39 (2%)	47	33

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	8	LYS
1	A	81	LEU
1	A	146	LEU
1	A	150	LEU
1	B	6	THR
1	B	67	LEU
1	B	81	LEU
1	B	93	LEU
1	B	146	LEU
1	B	150	LEU
1	B	152	LYS
1	C	146	LEU
1	C	150	LEU
1	D	82	LYS
1	D	93	LEU
1	D	146	LEU
1	D	150	LEU
1	D	152	LYS
1	E	8	LYS
1	E	150	LEU
1	E	152	LYS
1	F	81	LEU

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Mol	Chain	Res	Type
1	F	150	LEU
1	H	7	LEU
1	H	36	THR
1	H	93	LEU
1	H	146	LEU
1	H	150	LEU
1	I	67	LEU
1	I	150	LEU
1	J	81	LEU
1	J	82	LYS
1	K	7	LEU
1	K	81	LEU
1	K	150	LEU
1	L	4	THR
1	L	67	LEU
1	L	81	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	21	ASN
1	A	28	ASN
1	A	105	ASN
1	A	106	HIS
1	A	114	HIS
1	A	137	GLN
1	A	139	HIS
1	B	19	GLN
1	B	21	ASN
1	B	28	ASN
1	B	105	ASN
1	B	106	HIS
1	B	115	GLN
1	B	139	HIS
1	C	10	GLN
1	C	19	GLN
1	C	21	ASN
1	C	28	ASN
1	C	72	GLN
1	C	105	ASN
1	C	106	HIS

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Mol	Chain	Res	Type
1	C	115	GLN
1	C	139	HIS
1	D	19	GLN
1	D	21	ASN
1	D	28	ASN
1	D	51	GLN
1	D	105	ASN
1	D	106	HIS
1	D	139	HIS
1	E	10	GLN
1	E	19	GLN
1	E	21	ASN
1	E	28	ASN
1	E	92	GLN
1	E	105	ASN
1	E	106	HIS
1	E	115	GLN
1	E	137	GLN
1	E	139	HIS
1	F	19	GLN
1	F	21	ASN
1	F	28	ASN
1	F	105	ASN
1	G	19	GLN
1	G	28	ASN
1	G	72	GLN
1	G	105	ASN
1	H	19	GLN
1	H	21	ASN
1	H	28	ASN
1	H	72	GLN
1	H	92	GLN
1	H	105	ASN
1	H	115	GLN
1	H	137	GLN
1	I	19	GLN
1	I	21	ASN
1	I	28	ASN
1	I	92	GLN
1	I	105	ASN
1	J	19	GLN
1	J	21	ASN

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Mol	Chain	Res	Type
1	J	28	ASN
1	J	72	GLN
1	J	105	ASN
1	J	106	HIS
1	J	115	GLN
1	J	139	HIS
1	K	19	GLN
1	K	28	ASN
1	K	105	ASN
1	L	10	GLN
1	L	19	GLN
1	L	21	ASN
1	L	28	ASN
1	L	72	GLN
1	L	105	ASN
1	L	115	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	$\#\|Z\|>2$
4	PGE	C	1160	-	9,9,9	0.45	0	8,8,8	0.31	0
4	PGE	F	1159	-	9,9,9	0.44	0	8,8,8	0.28	0
4	PGE	H	1160	-	9,9,9	0.51	0	8,8,8	0.29	0
4	PGE	E	1160	-	9,9,9	0.40	0	8,8,8	0.40	0
4	PGE	L	1159	-	9,9,9	0.42	0	8,8,8	0.36	0
4	PGE	H	1159	-	9,9,9	0.43	0	8,8,8	0.28	0
3	PG4	C	1159	-	12,12,12	0.42	0	11,11,11	0.61	0
4	PGE	D	1159	-	9,9,9	0.44	0	8,8,8	0.38	0
4	PGE	B	1161	-	9,9,9	0.48	0	8,8,8	0.32	0
4	PGE	E	1159	-	9,9,9	0.48	0	8,8,8	0.76	0
4	PGE	F	1160	-	9,9,9	0.45	0	8,8,8	0.39	0
3	PG4	B	1159	-	12,12,12	0.50	0	11,11,11	0.28	0
4	PGE	B	1160	-	9,9,9	0.50	0	8,8,8	0.18	0
4	PGE	B	1162	-	9,9,9	0.46	0	8,8,8	0.30	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
4	PGE	C	1160	-	-	0/7/7/7	-
4	PGE	F	1159	-	-	5/7/7/7	-
4	PGE	H	1160	-	-	0/7/7/7	-
4	PGE	E	1160	-	-	2/7/7/7	-
4	PGE	L	1159	-	-	4/7/7/7	-
4	PGE	H	1159	-	-	6/7/7/7	-
3	PG4	C	1159	-	-	6/10/10/10	-
4	PGE	D	1159	-	-	0/7/7/7	-
4	PGE	B	1161	-	-	2/7/7/7	-
4	PGE	E	1159	-	-	4/7/7/7	-
4	PGE	F	1160	-	-	4/7/7/7	-
3	PG4	B	1159	-	-	2/10/10/10	-
4	PGE	B	1160	-	-	5/7/7/7	-
4	PGE	B	1162	-	-	3/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1160	PGE	O3-C5-C6-O4
3	C	1159	PG4	O2-C3-C4-O3
4	B	1160	PGE	O2-C3-C4-O3
4	B	1160	PGE	O1-C1-C2-O2
4	B	1162	PGE	O3-C5-C6-O4
4	F	1159	PGE	O3-C5-C6-O4
4	E	1159	PGE	O3-C5-C6-O4
4	H	1159	PGE	O3-C5-C6-O4
3	C	1159	PG4	O1-C1-C2-O2
4	F	1160	PGE	O2-C3-C4-O3
4	F	1160	PGE	O3-C5-C6-O4
4	H	1159	PGE	O1-C1-C2-O2
4	E	1159	PGE	O2-C3-C4-O3
4	B	1162	PGE	O2-C3-C4-O3
3	B	1159	PG4	O3-C5-C6-O4
4	L	1159	PGE	O3-C5-C6-O4
4	H	1159	PGE	O2-C3-C4-O3
4	H	1159	PGE	C4-C3-O2-C2
3	C	1159	PG4	C1-C2-O2-C3
4	L	1159	PGE	C6-C5-O3-C4
3	B	1159	PG4	C8-C7-O4-C6
4	L	1159	PGE	C4-C3-O2-C2
4	E	1159	PGE	C6-C5-O3-C4
4	H	1159	PGE	C3-C4-O3-C5
4	F	1159	PGE	C3-C4-O3-C5
4	L	1159	PGE	C3-C4-O3-C5
4	E	1160	PGE	C4-C3-O2-C2
3	C	1159	PG4	C6-C5-O3-C4
4	F	1160	PGE	C3-C4-O3-C5
4	E	1160	PGE	C3-C4-O3-C5
4	B	1161	PGE	C3-C4-O3-C5
4	F	1159	PGE	O2-C3-C4-O3
3	C	1159	PG4	O4-C7-C8-O5
3	C	1159	PG4	C8-C7-O4-C6
4	B	1161	PGE	O3-C5-C6-O4
4	F	1159	PGE	O1-C1-C2-O2
4	H	1159	PGE	C6-C5-O3-C4
4	F	1159	PGE	C4-C3-O2-C2
4	E	1159	PGE	C3-C4-O3-C5
4	B	1160	PGE	C4-C3-O2-C2
4	F	1160	PGE	C1-C2-O2-C3
4	B	1162	PGE	C3-C4-O3-C5

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Mol	Chain	Res	Type	Atoms
4	B	1160	PGE	C6-C5-O3-C4

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1160	PGE	1	0
4	L	1159	PGE	1	0
3	C	1159	PG4	5	0
4	E	1159	PGE	2	0
4	F	1160	PGE	1	0
4	B	1160	PGE	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, 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	155/158 (98%)	-0.37	2 (1%)	77	74	13, 15, 23, 37	0
1	B	154/158 (97%)	-0.49	1 (0%)	89	88	13, 15, 22, 32	0
1	C	157/158 (99%)	-0.46	3 (1%)	66	63	12, 15, 22, 35	0
1	D	154/158 (97%)	-0.43	1 (0%)	89	88	13, 15, 22, 33	0
1	E	154/158 (97%)	-0.36	1 (0%)	89	88	13, 15, 22, 32	0
1	F	156/158 (98%)	-0.46	1 (0%)	89	88	13, 15, 21, 24	0
1	G	154/158 (97%)	-0.40	3 (1%)	66	63	13, 16, 22, 38	0
1	H	154/158 (97%)	-0.42	3 (1%)	66	63	13, 15, 22, 34	0
1	I	154/158 (97%)	-0.38	2 (1%)	77	74	13, 15, 22, 35	0
1	J	153/158 (96%)	-0.36	5 (3%)	46	40	13, 16, 22, 38	0
1	K	153/158 (96%)	-0.44	2 (1%)	77	74	12, 15, 22, 31	0
1	L	155/158 (98%)	-0.46	1 (0%)	89	88	12, 15, 22, 32	0
All	All	1853/1896 (97%)	-0.42	25 (1%)	77	74	12, 15, 22, 38	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	5	THR	5.5
1	L	4	THR	4.7
1	A	7	LEU	4.7
1	J	6	THR	4.6
1	A	4	THR	4.3
1	G	5	THR	3.9
1	J	7	LEU	3.8
1	H	7	LEU	3.6
1	J	91	GLY	3.6
1	K	6	THR	3.5
1	G	6	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	K	7	LEU	3.1
1	D	5	THR	2.8
1	J	92	GLN	2.8
1	C	3	ALA	2.7
1	G	9	GLU	2.7
1	C	2	SER	2.7
1	I	8	LYS	2.5
1	E	6	THR	2.5
1	C	4	THR	2.5
1	J	9	GLU	2.4
1	H	92	GLN	2.3
1	B	5	THR	2.2
1	F	3	ALA	2.2
1	H	5	THR	2.1

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, 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	B-factors(Å^2)	Q<0.9
4	PGE	B	1160	10/10	0.81	0.17	36,39,42,42	0
4	PGE	H	1160	10/10	0.81	0.23	25,35,38,38	0
4	PGE	F	1160	10/10	0.83	0.18	39,43,46,46	0
4	PGE	H	1159	10/10	0.85	0.17	41,43,46,46	0
4	PGE	E	1159	10/10	0.86	0.17	22,26,28,33	0
4	PGE	L	1159	10/10	0.86	0.15	40,42,44,44	0
4	PGE	B	1161	10/10	0.88	0.16	41,42,46,47	0
4	PGE	B	1162	10/10	0.88	0.17	36,36,39,39	0
4	PGE	C	1160	10/10	0.88	0.16	36,38,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PG4	C	1159	13/13	0.88	0.17	32,35,39,39	0
4	PGE	F	1159	10/10	0.89	0.20	49,49,49,49	0
4	PGE	E	1160	10/10	0.90	0.15	42,44,46,47	0
3	PG4	B	1159	13/13	0.93	0.12	27,28,33,33	0
4	PGE	D	1159	10/10	0.96	0.12	17,26,32,34	0
2	CL	C	1161	1/1	1.00	0.04	15,15,15,15	0
2	CL	J	1159	1/1	1.00	0.03	14,14,14,14	0
2	CL	A	1159	1/1	1.00	0.05	14,14,14,14	0
2	CL	B	1163	1/1	1.00	0.04	14,14,14,14	0

6.5 Other polymers (i)

There are no such residues in this entry.