Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:51 AM GMT

PDB ID	:	2BW1
Title	:	IRON-BOUND CRYSTAL STRUCTURE OF DPS-LIKE PEROXIDE RESISTANCE PROTEIN (DPR) FROM STREPTOCOCCUS SUIS.
Authors	:	Kauko, A.; Pulliainen, A.; Haataja, S.; Finne, J.; Papageorgiou, A.C.
Deposited on	:	2005-07-07
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

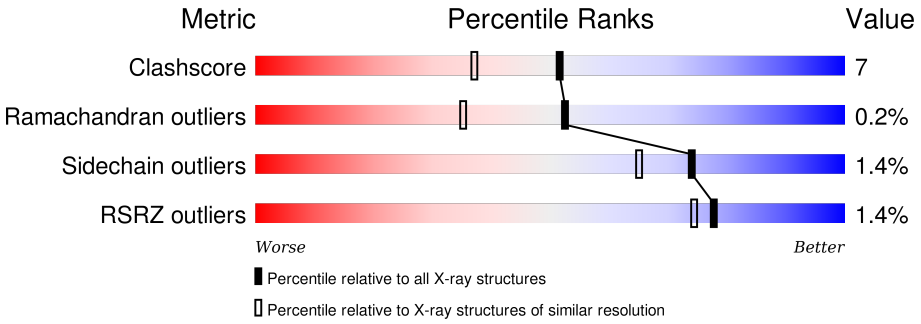
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.81 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))
Clashscore	102246	6347 (1.84-1.80)
Ramachandran outliers	100387	6276 (1.84-1.80)
Sidechain outliers	100360	6276 (1.84-1.80)
RSRZ outliers	91569	5439 (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 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	165	87% 5% 8%
1	B	165	85% 7% 8%
1	C	165	79% 12% 8%
1	D	165	82% 10% 8%
1	E	165	88% 8%
1	F	165	81% 10% 8%
1	G	165	4% 88% 11%

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Mol	Chain	Length	Quality of chain
1	H	165	2% 84% 8% 8%
1	I	165	% 85% 6% 8%
1	J	165	% 79% 10% 8%
1	K	165	% 83% 9% 7%
1	L	165	% 82% 9% 8%

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
2	EPE	D	200	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16600 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.

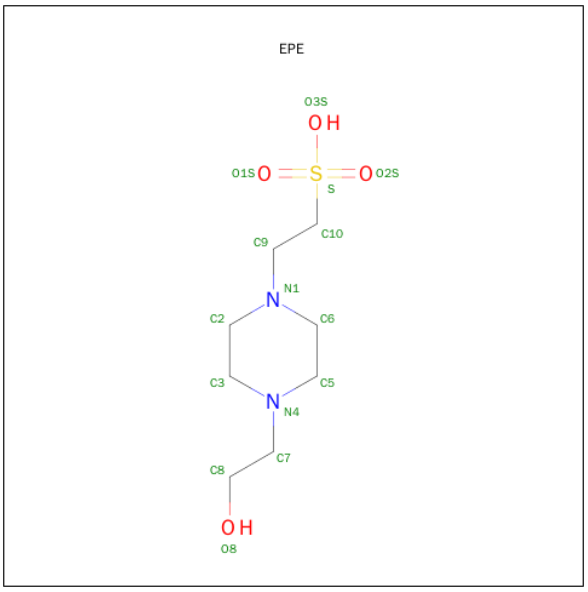
- Molecule 1 is a protein called DPS-LIKE PEROXIDE RESISTANCE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	151	Total	C	N	O	S	0	9	0
			1258	800	205	246	7			
1	B	151	Total	C	N	O	S	0	8	0
			1250	796	204	243	7			
1	C	151	Total	C	N	O	S	0	8	0
			1255	800	202	246	7			
1	D	152	Total	C	N	O	S	0	8	0
			1256	796	206	247	7			
1	E	151	Total	C	N	O	S	0	6	0
			1241	789	201	245	6			
1	F	151	Total	C	N	O	S	0	8	0
			1249	792	204	246	7			
1	G	165	Total	C	N	O	S	0	6	0
			1322	840	215	260	7			
1	H	151	Total	C	N	O	S	0	5	0
			1231	783	200	242	6			
1	I	151	Total	C	N	O	S	0	5	0
			1229	781	200	241	7			
1	J	151	Total	C	N	O	S	0	9	0
			1255	797	205	247	6			
1	K	153	Total	C	N	O	S	0	5	0
			1246	792	206	242	6			
1	L	151	Total	C	N	O	S	0	6	0
			1233	784	202	241	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	8	GLY	GLN	ENGINEERED MUTATION	UNP Q9F5J9

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O S 15 8 2 4 1	0	0
2	B	1	Total C N O S 15 8 2 4 1	0	0
2	C	1	Total C N O S 15 8 2 4 1	0	0
2	D	1	Total C N O S 15 8 2 4 1	0	0

- Molecule 3 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Fe 1 1	0	0
3	J	1	Total Fe 1 1	0	0
3	D	1	Total Fe 1 1	0	0
3	K	1	Total Fe 1 1	0	0
3	E	1	Total Fe 1 1	0	0
3	H	1	Total Fe 1 1	0	0
3	B	1	Total Fe 1 1	0	0
3	I	1	Total Fe 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Fe 1 1	0	0
3	A	1	Total Fe 1 1	0	0
3	L	1	Total Fe 1 1	0	0
3	F	1	Total Fe 1 1	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	K	1	Total Ca 1 1	0	0

- Molecule 5 is water.

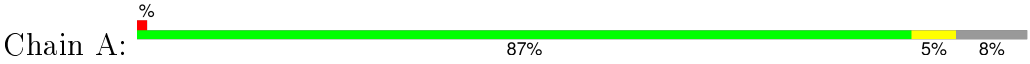
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	145	Total O 145 145	0	0
5	B	128	Total O 128 128	0	0
5	C	124	Total O 124 124	0	0
5	D	151	Total O 151 151	0	0
5	E	126	Total O 126 126	0	0
5	F	98	Total O 98 98	0	0
5	G	146	Total O 146 146	0	0
5	H	99	Total O 99 99	0	0
5	I	124	Total O 124 124	0	0
5	J	93	Total O 93 93	0	0
5	K	147	Total O 147 147	0	0
5	L	121	Total O 121 121	0	0

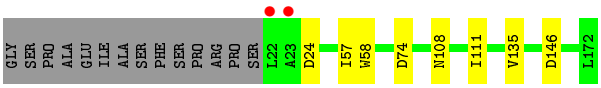
3 Residue-property plots (i)

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: DPS-LIKE PEROXIDE RESISTANCE PROTEIN

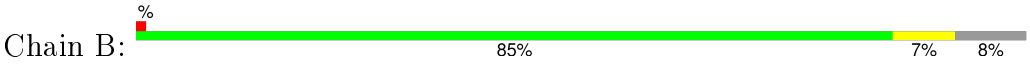
Chain A:

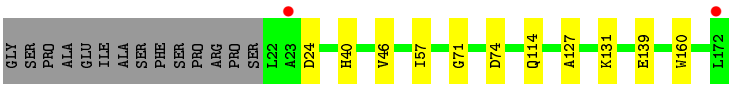




- Molecule 1: DPS-LIKE PEROXIDE RESISTANCE PROTEIN

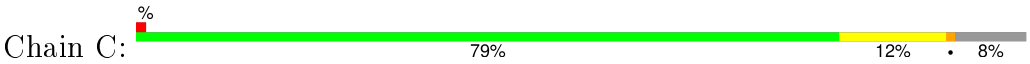
Chain B:





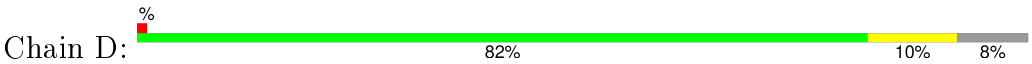
- Molecule 1: DPS-LIKE PEROXIDE RESISTANCE PROTEIN

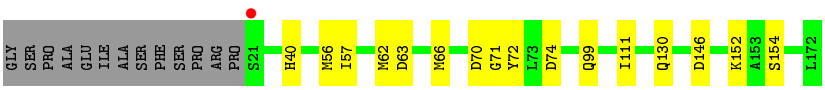
Chain C:



- Molecule 1: DPS-LIKE PEROXIDE RESISTANCE PROTEIN

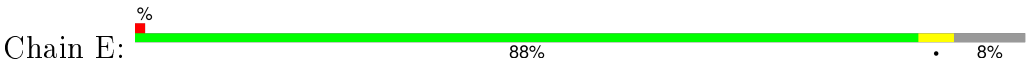
Chain D:

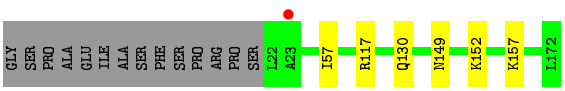




- Molecule 1: DPS-LIKE PEROXIDE RESISTANCE PROTEIN

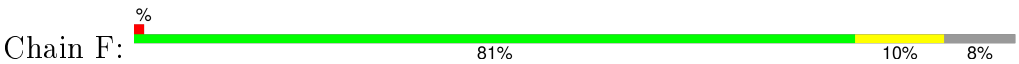
Chain E:

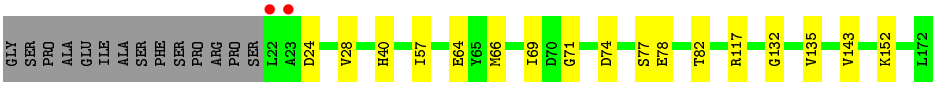




- Molecule 1: DPS-LIKE PEROXIDE RESISTANCE PROTEIN

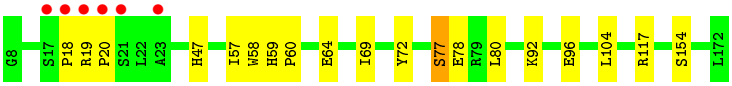
Chain F:





• Molecule 1: DPS-LIKE PEROXIDE RESISTANCE PROTEIN

Chain G:

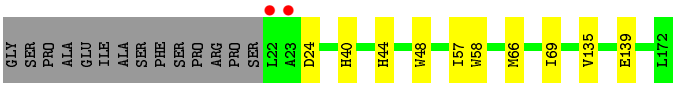


• Molecule 1: DPS-LIKE PEROXIDE RESISTANCE PROTEIN

Chain H:

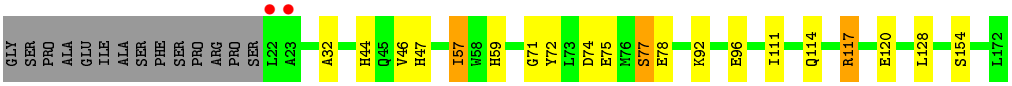
• Molecule 1: DPS-LIKE PEROXIDE RESISTANCE PROTEIN

Chain I:



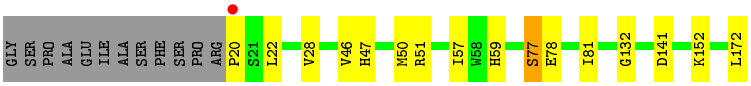
• Molecule 1: DPS-LIKE PEROXIDE RESISTANCE PROTEIN

Chain J:



• Molecule 1: DPS-LIKE PEROXIDE RESISTANCE PROTEIN

Chain K:



• Molecule 1: DPS-LIKE PEROXIDE RESISTANCE PROTEIN

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	105.13Å 138.05Å 142.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.53 – 1.81 19.53 – 1.81	Depositor EDS
% Data completeness (in resolution range)	98.3 (19.53-1.81) 99.3 (19.53-1.81)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	4.59 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.187 , 0.230 0.187 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	24.2	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 54.2	EDS
Estimated twinning fraction	0.024 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 188314 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16600	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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: CA, EPE, FE

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	0.66	0/1303	0.64	0/1759
1	B	0.66	0/1291	0.68	0/1743
1	C	1.24	2/1297 (0.2%)	0.68	0/1752
1	D	0.72	0/1297	0.68	0/1751
1	E	0.62	0/1275	0.65	0/1725
1	F	0.86	2/1290 (0.2%)	0.70	2/1743 (0.1%)
1	G	1.12	2/1361 (0.1%)	0.69	0/1839
1	H	0.64	0/1264	0.64	0/1710
1	I	0.70	0/1262	0.65	0/1706
1	J	1.03	2/1300 (0.2%)	0.59	0/1756
1	K	1.14	2/1279 (0.2%)	0.69	1/1728 (0.1%)
1	L	0.83	2/1264 (0.2%)	0.68	2/1707 (0.1%)
All	All	0.88	12/15483 (0.1%)	0.66	5/20919 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	77[A]	SER	C-N	26.91	1.96	1.34
1	C	77[B]	SER	C-N	26.91	1.96	1.34
1	G	77[A]	SER	C-N	23.63	1.88	1.34
1	G	77[B]	SER	C-N	23.63	1.88	1.34
1	K	77[A]	SER	C-N	22.62	1.86	1.34
1	K	77[B]	SER	C-N	22.62	1.86	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	77[A]	SER	C-N	21.00	1.82	1.34
1	J	77[B]	SER	C-N	21.00	1.82	1.34
1	F	77[A]	SER	C-N	14.17	1.66	1.34
1	F	77[B]	SER	C-N	14.17	1.66	1.34
1	L	77[A]	SER	C-N	12.52	1.62	1.34
1	L	77[B]	SER	C-N	12.52	1.62	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	77[A]	SER	O-C-N	-6.61	112.12	122.70
1	F	77[B]	SER	O-C-N	-6.61	112.12	122.70
1	L	77[A]	SER	O-C-N	-5.40	114.06	122.70
1	L	77[B]	SER	O-C-N	-5.40	114.06	122.70
1	K	51	ARG	NE-CZ-NH2	-5.12	117.74	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	20	PRO	Peptide

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	1258	0	1203	32	0
1	B	1250	0	1201	16	0
1	C	1255	0	1198	34	0
1	D	1256	0	1198	12	0
1	E	1241	0	1172	16	0
1	F	1249	0	1181	23	0
1	G	1322	0	1249	31	0
1	H	1231	0	1169	24	0
1	I	1229	0	1168	15	0
1	J	1255	0	1195	11	0
1	K	1246	0	1193	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1233	0	1169	29	0
2	A	15	0	17	0	0
2	B	15	0	17	1	0
2	C	15	0	17	0	0
2	D	15	0	17	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	L	1	0	0	0	0
4	K	1	0	0	0	0
5	A	145	0	0	2	0
5	B	128	0	0	3	0
5	C	124	0	0	1	0
5	D	151	0	0	3	0
5	E	126	0	0	4	0
5	F	98	0	0	3	0
5	G	146	0	0	3	0
5	H	99	0	0	0	0
5	I	124	0	0	0	0
5	J	93	0	0	0	0
5	K	147	0	0	0	0
5	L	121	0	0	4	0
All	All	16600	0	14364	201	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (201) 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:57[B]:ILE:HD11	1:L:57[B]:ILE:CG1	1.26	1.62
1:A:57[B]:ILE:CD1	1:H:57[B]:ILE:HD11	1.24	1.56
1:C:77[B]:SER:C	1:C:78[B]:GLU:CA	1.86	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57[B]:ILE:HD11	1:F:57[B]:ILE:CD1	1.47	1.42
1:C:57[B]:ILE:CD1	1:L:57[B]:ILE:HG13	1.47	1.41
1:B:57[B]:ILE:CD1	1:F:57[B]:ILE:HD11	1.52	1.39
1:G:77[B]:SER:C	1:G:78[B]:GLU:CA	1.95	1.33
1:J:77[A]:SER:C	1:J:78[A]:GLU:N	1.82	1.31
1:A:57[B]:ILE:CD1	1:K:57[B]:ILE:HD11	1.59	1.31
1:K:77[B]:SER:C	1:K:78[B]:GLU:CA	1.97	1.30
1:C:57[B]:ILE:HD11	1:L:57[B]:ILE:CD1	1.58	1.30
1:A:57[B]:ILE:CG1	1:K:57[B]:ILE:HD11	1.60	1.30
1:C:77[B]:SER:CA	1:C:78[B]:GLU:N	1.92	1.29
1:K:77[A]:SER:C	1:K:78[A]:GLU:N	1.86	1.29
1:G:77[A]:SER:C	1:G:78[A]:GLU:N	1.88	1.25
1:G:77[B]:SER:CA	1:G:78[B]:GLU:N	2.01	1.24
1:A:57[B]:ILE:HD11	1:H:57[B]:ILE:CD1	1.68	1.23
1:A:57[B]:ILE:CD1	1:K:57[B]:ILE:CG1	2.18	1.22
1:A:57[B]:ILE:CD1	1:H:57[B]:ILE:CD1	2.17	1.21
1:K:77[B]:SER:CA	1:K:78[B]:GLU:N	2.04	1.20
1:A:57[B]:ILE:HD11	1:K:57[B]:ILE:CG1	1.71	1.19
1:A:57[B]:ILE:CD1	1:K:57[B]:ILE:CD1	2.20	1.19
1:C:77[A]:SER:C	1:C:78[A]:GLU:N	1.95	1.18
1:C:57[B]:ILE:CD1	1:L:57[B]:ILE:CG1	2.09	1.15
1:A:57[B]:ILE:HG12	1:K:57[B]:ILE:HD11	1.24	1.14
1:A:57[B]:ILE:HD11	1:K:57[B]:ILE:CD1	1.78	1.14
1:K:77[B]:SER:O	1:K:78[B]:GLU:N	1.79	1.13
1:C:77[B]:SER:O	1:C:78[B]:GLU:N	1.79	1.12
1:C:57[B]:ILE:CD1	1:L:57[B]:ILE:CD1	2.25	1.11
1:E:57:ILE:HD11	1:L:57[B]:ILE:HD11	1.14	1.10
1:G:77[B]:SER:O	1:G:78[B]:GLU:N	1.83	1.09
1:B:57[B]:ILE:CD1	1:F:57[B]:ILE:CD1	2.17	1.09
1:A:24:ASP:HB3	1:A:135:VAL:HG11	1.36	1.07
1:A:57[B]:ILE:HD13	1:K:57[B]:ILE:HG12	1.33	1.06
1:G:57[B]:ILE:CG2	1:I:57[B]:ILE:HD11	1.84	1.06
1:B:57[B]:ILE:HG13	1:F:57[B]:ILE:HD13	1.34	1.05
1:A:57[B]:ILE:HD11	1:K:57[B]:ILE:HG13	1.39	1.03
1:A:57[B]:ILE:CG1	1:H:57[B]:ILE:HD11	1.89	1.01
1:A:57[B]:ILE:HG13	1:H:57[B]:ILE:HD13	1.43	1.00
1:E:57:ILE:CD1	1:L:57[B]:ILE:HD11	1.93	0.99
1:G:57[B]:ILE:HG21	1:I:57[B]:ILE:HD11	1.45	0.97
1:C:77[B]:SER:O	1:C:78[B]:GLU:CA	2.08	0.97
1:B:57[B]:ILE:CG1	1:F:57[B]:ILE:HD13	1.95	0.97
1:G:57[B]:ILE:CG2	1:I:57[B]:ILE:CD1	2.43	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57[B]:ILE:CG1	1:H:57[B]:ILE:CD1	2.43	0.96
1:C:57[B]:ILE:HD11	1:L:57[B]:ILE:HG13	1.03	0.96
1:C:57[B]:ILE:HD13	1:L:57[B]:ILE:HG13	1.45	0.95
1:C:57[B]:ILE:CD1	1:L:57[B]:ILE:HD11	1.93	0.95
1:C:57[B]:ILE:HD11	1:L:57[B]:ILE:HD11	1.45	0.95
1:A:57[B]:ILE:HD11	1:K:57[B]:ILE:HD11	1.41	0.94
1:A:57[B]:ILE:HG13	1:H:57[B]:ILE:CD1	1.97	0.94
1:L:74[A]:ASP:C	1:L:75[A]:GLU:N	2.19	0.94
1:B:57[B]:ILE:CG1	1:F:57[B]:ILE:CD1	2.44	0.94
1:A:57[B]:ILE:HD13	1:K:57[B]:ILE:CG1	1.90	0.93
1:A:24:ASP:HB3	1:A:135:VAL:CG1	1.99	0.92
1:K:77[B]:SER:O	1:K:78[B]:GLU:CA	2.15	0.92
1:G:77[B]:SER:C	1:G:78[B]:GLU:N	0.81	0.85
1:K:77[B]:SER:C	1:K:78[B]:GLU:N	0.81	0.85
1:G:77[B]:SER:O	1:G:78[B]:GLU:CA	2.20	0.85
1:F:57[B]:ILE:HG13	1:J:57:ILE:HD13	1.58	0.85
1:C:57[B]:ILE:HG13	1:E:57:ILE:HD11	1.58	0.83
1:A:57[B]:ILE:HG12	1:K:57[B]:ILE:CD1	2.08	0.82
1:C:57[B]:ILE:HG13	1:E:57:ILE:CD1	2.10	0.82
1:C:57[B]:ILE:HD11	1:L:57[B]:ILE:HG12	1.56	0.81
1:C:77[B]:SER:C	1:C:78[B]:GLU:N	0.73	0.79
1:E:157:LYS:NZ	5:E:2116:HOH:O	2.17	0.78
1:C:77[B]:SER:O	1:C:78[B]:GLU:HA	1.82	0.78
1:H:57[B]:ILE:HD11	1:K:57[B]:ILE:HD11	1.67	0.77
1:J:72:TYR:HH	1:J:154[B]:SER:HG	1.29	0.77
1:D:63[A]:ASP:OD2	5:D:2045:HOH:O	2.01	0.76
1:A:57[B]:ILE:HD11	1:H:57[B]:ILE:HD11	0.76	0.75
1:G:57[B]:ILE:HG22	1:I:57[B]:ILE:CD1	2.15	0.75
2:B:200:EPE:H51	5:B:2127:HOH:O	1.85	0.75
1:C:77[B]:SER:C	1:C:78[B]:GLU:HA	2.05	0.75
1:F:152:LYS:HE3	5:F:2074:HOH:O	1.87	0.74
1:A:57[B]:ILE:CD1	1:K:57[B]:ILE:HG12	1.98	0.72
1:F:152:LYS:CE	5:F:2074:HOH:O	2.37	0.72
1:C:57[B]:ILE:HD12	1:L:57[B]:ILE:CD1	2.18	0.71
1:L:24:ASP:HB3	1:L:135:VAL:CG1	2.19	0.71
1:H:22:LEU:HD21	1:H:141:ASP:HB2	1.74	0.70
1:A:57[B]:ILE:HD12	1:H:57[B]:ILE:HD11	1.59	0.70
1:F:57[B]:ILE:CG1	1:J:57:ILE:HD13	2.23	0.69
1:K:77[B]:SER:O	1:K:78[B]:GLU:HA	1.91	0.69
1:D:146:ASP:OD1	5:D:2127:HOH:O	2.11	0.68
1:A:57[B]:ILE:HD13	1:K:57[B]:ILE:CD1	2.18	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:57[B]:ILE:CG2	1:I:57[B]:ILE:HD13	2.24	0.68
1:C:40:HIS:CE1	1:C:66[B]:MET:SD	2.88	0.67
1:D:57:ILE:HD11	1:G:57[A]:ILE:HD13	1.77	0.67
1:A:108:ASN:HB2	5:A:2094:HOH:O	1.93	0.67
1:D:57:ILE:CD1	1:G:57[A]:ILE:HD13	2.24	0.66
1:H:57[B]:ILE:HD11	1:K:57[B]:ILE:CD1	2.26	0.66
1:B:57[B]:ILE:CG1	1:F:57[B]:ILE:HD11	2.14	0.65
1:E:57:ILE:HD11	1:L:57[B]:ILE:CD1	2.09	0.65
1:D:72:TYR:HH	1:D:154[B]:SER:HG	1.39	0.64
1:L:117:ARG:HG3	5:L:2089:HOH:O	1.96	0.64
1:G:77[B]:SER:O	1:G:78[B]:GLU:HA	1.95	0.63
1:B:57[B]:ILE:HD11	1:F:57[B]:ILE:HD11	0.69	0.63
1:B:71:GLY:O	1:B:74[B]:ASP:HB2	1.98	0.62
1:C:57[B]:ILE:CG1	1:E:57:ILE:HD11	2.28	0.62
1:F:24:ASP:HB3	1:F:135:VAL:HG11	1.81	0.62
1:B:24:ASP:HB2	1:B:139:GLU:OE2	2.00	0.62
1:L:24:ASP:HB3	1:L:135:VAL:HG13	1.82	0.61
1:H:22:LEU:CD2	1:H:141:ASP:HB2	2.30	0.61
1:L:152:LYS:HE3	5:L:2096:HOH:O	1.99	0.61
1:H:24:ASP:HB3	1:H:135:VAL:CG1	2.31	0.61
1:B:127:ALA:O	1:B:131:LYS:HG3	2.01	0.60
1:C:130:GLN:OE1	1:C:152:LYS:HE3	2.02	0.60
1:H:24:ASP:HB3	1:H:135:VAL:HG11	1.83	0.60
1:G:92:LYS:HD3	5:G:2033:HOH:O	2.01	0.59
1:J:117[B]:ARG:NH1	1:J:120:GLU:HB2	2.17	0.59
1:I:40:HIS:CE1	1:I:66[B]:MET:HG2	2.39	0.57
1:L:24:ASP:HB3	1:L:135:VAL:HG11	1.84	0.57
1:C:68:GLU:OE2	1:C:72[B]:TYR:OH	2.13	0.57
1:F:24:ASP:HB3	1:F:135:VAL:CG1	2.37	0.55
1:H:57[B]:ILE:CD1	1:K:57[B]:ILE:HD11	2.36	0.55
1:A:57[B]:ILE:CD1	1:K:57[B]:ILE:HG13	2.10	0.55
1:C:92:LYS:O	1:C:96:GLU:HG3	2.07	0.54
1:J:92:LYS:NZ	1:J:96:GLU:OE1	2.41	0.54
1:C:135:VAL:O	1:C:139:GLU:HG3	2.07	0.54
1:A:24:ASP:CB	1:A:135:VAL:CG1	2.81	0.53
1:E:57:ILE:CD1	1:L:57[B]:ILE:CD1	2.77	0.53
1:G:92:LYS:NZ	1:G:96:GLU:OE1	2.41	0.53
1:C:152:LYS:CE	5:C:2100:HOH:O	2.56	0.53
1:I:24:ASP:HB3	1:I:135:VAL:CG1	2.38	0.53
1:G:59:HIS:HB3	1:G:60:PRO:HD3	1.92	0.52
1:C:77[B]:SER:N	1:C:78[B]:GLU:N	2.54	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:57[B]:ILE:HG22	1:I:57[B]:ILE:HD13	1.86	0.51
1:L:71:GLY:O	1:L:74[B]:ASP:HB2	2.10	0.51
1:L:75[A]:GLU:OE2	5:L:2053:HOH:O	2.19	0.50
1:C:57[B]:ILE:CD1	1:E:57:ILE:HD11	2.42	0.50
1:K:28:VAL:HG11	1:K:132:GLY:HA2	1.94	0.50
1:D:40:HIS:CD2	1:D:70:ASP:OD2	2.65	0.50
1:H:57[B]:ILE:CG1	1:K:57[B]:ILE:HD12	2.42	0.50
1:G:117:ARG:HG3	5:G:2106:HOH:O	2.12	0.50
1:J:71:GLY:O	1:J:74[B]:ASP:HB2	2.12	0.49
1:G:57[B]:ILE:HG23	1:I:57[B]:ILE:CD1	2.40	0.49
1:D:71:GLY:O	1:D:74[B]:ASP:HB2	2.12	0.49
1:B:40:HIS:HE1	5:B:2015:HOH:O	1.94	0.49
1:G:77[B]:SER:N	1:G:78[B]:GLU:N	2.59	0.49
1:L:152:LYS:CE	5:L:2096:HOH:O	2.60	0.49
1:H:71:GLY:O	1:H:74[B]:ASP:HB2	2.13	0.49
1:D:57:ILE:HD13	1:G:57[A]:ILE:HD13	1.95	0.49
1:J:117[B]:ARG:HH12	1:J:120:GLU:HB2	1.77	0.48
1:H:57[B]:ILE:CG1	1:K:57[B]:ILE:CD1	2.90	0.48
1:H:57[B]:ILE:HG12	1:K:57[B]:ILE:HD12	1.95	0.48
1:B:160:TRP:CH2	1:L:78[A]:GLU:HG2	2.48	0.48
1:G:47:HIS:CE1	1:G:59:HIS:CE1	3.01	0.48
1:B:57[B]:ILE:CD1	1:F:57[B]:ILE:HD13	2.19	0.48
1:I:40:HIS:ND1	1:I:66[B]:MET:HG2	2.29	0.48
1:E:117:ARG:HD3	5:E:2097:HOH:O	2.12	0.48
1:I:135:VAL:O	1:I:139:GLU:HG3	2.14	0.47
1:H:47:HIS:CE1	1:H:59:HIS:CE1	3.02	0.47
1:C:71:GLY:O	1:C:74[B]:ASP:HB2	2.13	0.47
1:K:46:VAL:O	1:K:50:MET:HB2	2.15	0.46
1:L:74[B]:ASP:O	1:L:78[B]:GLU:HB2	2.14	0.46
1:A:57[B]:ILE:HD12	1:H:57[B]:ILE:CD1	2.29	0.46
1:G:77[B]:SER:C	1:G:78[B]:GLU:HA	2.14	0.46
1:G:57[B]:ILE:HD11	1:G:58:TRP:CE2	2.51	0.45
1:F:74[B]:ASP:O	1:F:78[B]:GLU:HB2	2.15	0.45
1:I:24:ASP:HB3	1:I:135:VAL:HG11	1.99	0.45
1:E:130:GLN:OE1	1:E:152:LYS:HE3	2.16	0.45
1:I:57[A]:ILE:HG23	1:I:58:TRP:CD1	2.52	0.45
1:G:64:GLU:OE2	5:G:2052:HOH:O	2.20	0.45
1:A:74[B]:ASP:HB2	5:A:2057:HOH:O	2.16	0.44
1:L:110:THR:OG1	1:L:113:GLU:HG3	2.17	0.44
1:D:56:MET:CG	1:G:57[B]:ILE:HD13	2.48	0.44
2:D:200:EPE:H51	5:D:2149:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:32:ALA:HA	1:J:128:LEU:HD21	2.00	0.44
1:B:40:HIS:ND1	5:B:2011:HOH:O	1.93	0.43
1:E:152:LYS:CE	5:E:2104:HOH:O	2.65	0.43
1:C:57[B]:ILE:HG13	1:E:57:ILE:HD13	1.97	0.43
1:D:72:TYR:OH	1:D:154[B]:SER:OG	2.16	0.43
1:G:72:TYR:HH	1:G:154[B]:SER:HB3	1.82	0.43
1:L:47:HIS:CE1	1:L:59:HIS:CE1	3.07	0.42
1:A:146:ASP:OD1	1:E:149:ASN:ND2	2.52	0.42
1:F:82:THR:HG22	1:K:172:LEU:HD11	2.01	0.42
1:G:59:HIS:HB3	1:G:60:PRO:CD	2.49	0.42
1:F:28:VAL:HG11	1:F:132:GLY:HA2	2.00	0.42
1:C:57[A]:ILE:HG23	1:C:58:TRP:CD1	2.54	0.42
1:D:62:MET:O	1:D:66[B]:MET:HG3	2.19	0.42
1:K:47:HIS:CE1	1:K:59:HIS:CE1	3.08	0.42
1:F:143:VAL:HG23	1:K:152:LYS:HE3	2.02	0.42
1:G:77[A]:SER:O	1:G:80:LEU:HB3	2.20	0.41
1:I:40:HIS:CE1	1:I:66[B]:MET:SD	3.13	0.41
1:F:71:GLY:O	1:F:74[B]:ASP:HB2	2.20	0.41
1:D:130:GLN:OE1	1:D:152:LYS:HE3	2.20	0.41
1:F:64:GLU:OE2	5:F:2032:HOH:O	2.22	0.41
1:I:48:TRP:HB3	1:K:81:ILE:HD11	2.03	0.41
1:F:40:HIS:CE1	1:F:66[B]:MET:SD	3.14	0.41
1:H:57[B]:ILE:CD1	1:K:57[B]:ILE:CD1	2.95	0.40
1:B:46:VAL:HG13	1:B:114:GLN:HB3	2.04	0.40
1:J:47:HIS:CE1	1:J:59:HIS:CE1	3.09	0.40
1:E:57:ILE:CG1	1:L:57[B]:ILE:HD11	2.47	0.40
1:H:22:LEU:HD23	1:H:139:GLU:HB3	2.02	0.40
1:E:152:LYS:HE3	5:E:2104:HOH:O	2.22	0.40
1:J:46:VAL:HG13	1:J:114:GLN:HB3	2.04	0.40
1:F:117[B]:ARG:HE	1:F:117[B]:ARG:HB2	1.71	0.40
1:C:47:HIS:CE1	1:C:59:HIS:CE1	3.10	0.40
1:A:57[A]:ILE:HG23	1:A:58:TRP:CD1	2.57	0.40
1:K:22:LEU:HD22	1:K:141:ASP:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	158/165 (96%)	157 (99%)	1 (1%)	0	100 100
1	B	157/165 (95%)	156 (99%)	1 (1%)	0	100 100
1	C	157/165 (95%)	154 (98%)	3 (2%)	0	100 100
1	D	158/165 (96%)	157 (99%)	1 (1%)	0	100 100
1	E	155/165 (94%)	154 (99%)	1 (1%)	0	100 100
1	F	157/165 (95%)	156 (99%)	1 (1%)	0	100 100
1	G	169/165 (102%)	162 (96%)	4 (2%)	3 (2%)	11 2
1	H	154/165 (93%)	153 (99%)	1 (1%)	0	100 100
1	I	154/165 (93%)	150 (97%)	4 (3%)	0	100 100
1	J	158/165 (96%)	156 (99%)	2 (1%)	0	100 100
1	K	156/165 (94%)	155 (99%)	1 (1%)	0	100 100
1	L	155/165 (94%)	154 (99%)	1 (1%)	0	100 100
All	All	1888/1980 (95%)	1864 (99%)	21 (1%)	3 (0%)	52 35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	18	PRO
1	G	19	ARG
1	G	20	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	136/140 (97%)	135 (99%)	1 (1%)	88 85
1	B	135/140 (96%)	135 (100%)	0	100 100
1	C	136/140 (97%)	130 (96%)	6 (4%)	35 16
1	D	136/140 (97%)	134 (98%)	2 (2%)	72 62
1	E	132/140 (94%)	132 (100%)	0	100 100
1	F	134/140 (96%)	133 (99%)	1 (1%)	88 85
1	G	140/140 (100%)	138 (99%)	2 (1%)	74 65
1	H	131/140 (94%)	128 (98%)	3 (2%)	58 42
1	I	131/140 (94%)	129 (98%)	2 (2%)	72 62
1	J	136/140 (97%)	128 (94%)	8 (6%)	24 8
1	K	133/140 (95%)	133 (100%)	0	100 100
1	L	131/140 (94%)	130 (99%)	1 (1%)	86 83
All	All	1611/1680 (96%)	1585 (98%)	26 (2%)	74 59

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	ILE
1	C	74[A]	ASP
1	C	74[B]	ASP
1	C	75[A]	GLU
1	C	75[B]	GLU
1	C	101	LYS
1	C	160	TRP
1	D	99	GLN
1	D	111	ILE
1	F	69	ILE
1	G	69	ILE
1	G	104	LEU
1	H	69	ILE
1	H	117	ARG
1	H	146	ASP
1	I	44	HIS
1	I	69	ILE
1	J	44	HIS
1	J	57	ILE
1	J	75[A]	GLU
1	J	75[B]	GLU
1	J	111[A]	ILE

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Mol	Chain	Res	Type
1	J	111[B]	ILE
1	J	117[A]	ARG
1	J	117[B]	ARG
1	L	95	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	C	99	GLN
1	F	99	GLN
1	I	99	GLN
1	J	99	GLN
1	J	145	ASN
1	K	130	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 carbohydrates in this entry.

5.6 Ligand geometry

Of 17 ligands modelled in this entry, 13 are monoatomic - leaving 4 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	$\#\|Z\|>2$
2	EPE	A	200	-	14,15,15	0.48	0	18,20,20	2.90	7 (38%)
2	EPE	B	200	-	14,15,15	0.56	0	18,20,20	3.79	7 (38%)
2	EPE	C	200	-	14,15,15	0.43	0	18,20,20	2.49	7 (38%)
2	EPE	D	200	-	14,15,15	0.70	1 (7%)	18,20,20	2.23	7 (38%)

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
2	EPE	A	200	-	-	0/9/19/19	0/1/1/1
2	EPE	B	200	-	-	0/9/19/19	0/1/1/1
2	EPE	C	200	-	-	0/9/19/19	0/1/1/1
2	EPE	D	200	-	-	0/9/19/19	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	200	EPE	O3S-S	-2.06	1.41	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	200	EPE	O2S-S-C10	-6.60	101.27	106.91
2	C	200	EPE	O2S-S-C10	-5.13	102.53	106.91
2	A	200	EPE	O2S-S-C10	-5.07	102.58	106.91
2	D	200	EPE	C5-C6-N1	-3.37	104.60	110.63
2	C	200	EPE	O3S-S-O1S	-2.62	105.51	111.61
2	B	200	EPE	C9-N1-C2	-2.61	104.57	111.27
2	C	200	EPE	C6-N1-C2	2.26	113.79	108.90
2	C	200	EPE	C2-C3-N4	2.32	114.79	110.63
2	D	200	EPE	C6-N1-C2	2.39	114.07	108.90
2	B	200	EPE	C7-N4-C5	2.67	118.11	111.27
2	D	200	EPE	C2-C3-N4	2.77	115.58	110.63
2	D	200	EPE	C3-C2-N1	2.77	115.59	110.63
2	A	200	EPE	C9-C10-S	2.87	121.39	112.51
2	D	200	EPE	C7-N4-C3	2.91	118.73	111.27
2	B	200	EPE	C6-N1-C2	2.98	115.36	108.90
2	A	200	EPE	C6-N1-C2	3.14	115.71	108.90
2	C	200	EPE	C7-N4-C3	3.15	119.33	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	200	EPE	C7-N4-C5	3.27	119.66	111.27
2	D	200	EPE	C7-N4-C5	3.46	120.13	111.27
2	A	200	EPE	C7-N4-C3	3.57	120.42	111.27
2	B	200	EPE	C7-N4-C3	3.74	120.84	111.27
2	C	200	EPE	C5-N4-C3	4.16	117.91	108.90
2	A	200	EPE	C5-N4-C3	4.70	119.08	108.90
2	B	200	EPE	C5-N4-C3	4.78	119.25	108.90
2	D	200	EPE	C5-N4-C3	5.09	119.92	108.90
2	C	200	EPE	O1S-S-C10	5.71	111.78	106.91
2	A	200	EPE	O1S-S-C10	7.64	113.43	106.91
2	B	200	EPE	O1S-S-C10	12.03	117.17	106.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	200	EPE	1	0
2	D	200	EPE	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	151/165 (91%)	-0.35	2 (1%)	79	76	16, 20, 29, 39	0
1	B	151/165 (91%)	-0.28	2 (1%)	79	76	16, 21, 29, 43	0
1	C	151/165 (91%)	-0.25	2 (1%)	79	76	18, 22, 32, 43	0
1	D	152/165 (92%)	-0.30	1 (0%)	89	87	16, 20, 29, 42	0
1	E	151/165 (91%)	-0.24	1 (0%)	89	87	19, 23, 32, 42	0
1	F	151/165 (91%)	-0.10	2 (1%)	79	76	20, 24, 35, 43	0
1	G	165/165 (100%)	-0.13	6 (3%)	46	40	17, 23, 35, 49	0
1	H	151/165 (91%)	-0.04	3 (1%)	68	64	19, 26, 37, 50	0
1	I	151/165 (91%)	-0.16	2 (1%)	79	76	17, 22, 31, 39	0
1	J	151/165 (91%)	-0.01	2 (1%)	79	76	20, 25, 34, 42	0
1	K	153/165 (92%)	-0.20	1 (0%)	89	87	17, 22, 31, 41	0
1	L	151/165 (91%)	-0.19	2 (1%)	79	76	20, 24, 31, 37	0
All	All	1829/1980 (92%)	-0.19	26 (1%)	78	74	16, 23, 33, 50	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	22	LEU	5.5
1	D	21	SER	5.4
1	G	18	PRO	5.2
1	A	22	LEU	4.7
1	J	22	LEU	4.5
1	K	20	PRO	4.2
1	C	23	ALA	3.9
1	H	23	ALA	3.8
1	G	19	ARG	3.8
1	L	22	LEU	3.7
1	I	23	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	172	LEU	3.6
1	F	23	ALA	3.5
1	L	23	ALA	3.4
1	B	23	ALA	3.1
1	A	23	ALA	3.0
1	G	17	SER	2.8
1	H	22	LEU	2.8
1	G	20	PRO	2.8
1	F	22	LEU	2.7
1	E	23	ALA	2.6
1	G	23	ALA	2.3
1	J	23	ALA	2.2
1	H	104	LEU	2.2
1	G	21	SER	2.2
1	C	22	LEU	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 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
2	EPE	D	200	15/15	0.95	0.15	2.37	25,32,37,37	0
2	EPE	A	200	15/15	0.94	0.16	1.49	26,39,47,50	0
2	EPE	C	200	15/15	0.95	0.13	1.45	28,35,43,45	0
2	EPE	B	200	15/15	0.97	0.11	0.87	22,29,38,40	0
4	CA	K	1501	1/1	0.98	0.06	-1.59	25,25,25,25	0
3	FE	G	2000	1/1	0.96	0.06	-1.65	26,26,26,26	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	FE	J	2000	1/1	0.99	0.04	-1.76	23,23,23,23	1
3	FE	K	2000	1/1	0.98	0.03	-1.87	24,24,24,24	1
3	FE	L	2000	1/1	0.94	0.06	-1.88	31,31,31,31	1
3	FE	I	2000	1/1	0.98	0.04	-1.94	26,26,26,26	1
3	FE	F	2000	1/1	0.97	0.07	-2.00	27,27,27,27	1
3	FE	B	2000	1/1	0.97	0.05	-2.01	24,24,24,24	1
3	FE	C	2000	1/1	0.97	0.06	-2.10	26,26,26,26	1
3	FE	H	2000	1/1	0.98	0.04	-2.28	26,26,26,26	1
3	FE	D	2000	1/1	0.98	0.03	-2.36	26,26,26,26	1
3	FE	A	2000	1/1	0.97	0.04	-2.44	25,25,25,25	1
3	FE	E	2000	1/1	0.98	0.05	-2.81	26,26,26,26	1

6.5 Other polymers (i)

There are no such residues in this entry.