Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:29 PM GMT

PDB ID	:	1XE3
Title	:	Crystal Structure of purine nucleoside phosphorylase DeoD from Bacillus anthracis
Authors	:	Grenha, R.; Levdikov, V.M.; Fogg, M.; Blagova, E.V.; Brannigan, J.A.; Wilkinson, A.J.; Wilson, K.S.; Structural Proteomics in Europe (SPINE)
Deposited on	:	2004-09-09
Resolution	:	2.24 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:

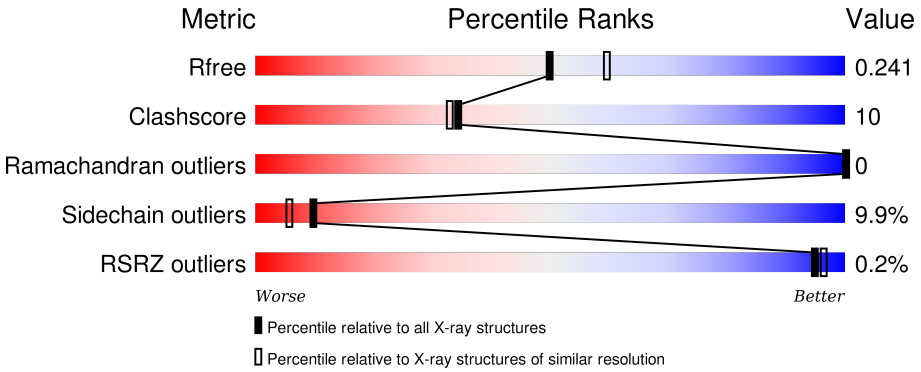
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.24 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	1611 (2.26-2.22)
Clashscore	102246	1764 (2.26-2.22)
Ramachandran outliers	100387	1724 (2.26-2.22)
Sidechain outliers	100360	1724 (2.26-2.22)
RSRZ outliers	91569	1616 (2.26-2.22)

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	245	73% 18% • 5%
1	B	245	76% 13% 6% 5%
1	C	245	77% 14% 5% •
1	D	245	72% 18% 6% •
1	E	245	% 75% 16% • •

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Mol	Chain	Length	Quality of chain
1	F	245	77% 13% 5% 5%

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	CL	C	806	-	-	X	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11450 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 purine nucleoside phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1782	1127	296	347	12			
1	B	233	Total	C	N	O	S	0	0	0
			1780	1127	294	347	12			
1	C	234	Total	C	N	O	S	0	0	0
			1790	1133	297	348	12			
1	D	235	Total	C	N	O	S	0	0	0
			1799	1138	299	350	12			
1	E	234	Total	C	N	O	S	0	0	0
			1789	1132	296	349	12			
1	F	233	Total	C	N	O	S	0	1	0
			1788	1132	297	347	12			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	MET	-	CLONING ARTIFACT	UNP Q81T09
A	-8	GLY	-	CLONING ARTIFACT	UNP Q81T09
A	-7	SER	-	CLONING ARTIFACT	UNP Q81T09
A	-6	SER	-	CLONING ARTIFACT	UNP Q81T09
A	-5	HIS	-	EXPRESSION TAG	UNP Q81T09
A	-4	HIS	-	EXPRESSION TAG	UNP Q81T09
A	-3	HIS	-	EXPRESSION TAG	UNP Q81T09
A	-2	HIS	-	EXPRESSION TAG	UNP Q81T09
A	-1	HIS	-	EXPRESSION TAG	UNP Q81T09
A	0	HIS	-	EXPRESSION TAG	UNP Q81T09
B	-9	MET	-	CLONING ARTIFACT	UNP Q81T09
B	-8	GLY	-	CLONING ARTIFACT	UNP Q81T09
B	-7	SER	-	CLONING ARTIFACT	UNP Q81T09
B	-6	SER	-	CLONING ARTIFACT	UNP Q81T09
B	-5	HIS	-	EXPRESSION TAG	UNP Q81T09
B	-4	HIS	-	EXPRESSION TAG	UNP Q81T09
B	-3	HIS	-	EXPRESSION TAG	UNP Q81T09

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	EXPRESSION TAG	UNP Q81T09
B	-1	HIS	-	EXPRESSION TAG	UNP Q81T09
B	0	HIS	-	EXPRESSION TAG	UNP Q81T09
C	-9	MET	-	CLONING ARTIFACT	UNP Q81T09
C	-8	GLY	-	CLONING ARTIFACT	UNP Q81T09
C	-7	SER	-	CLONING ARTIFACT	UNP Q81T09
C	-6	SER	-	CLONING ARTIFACT	UNP Q81T09
C	-5	HIS	-	EXPRESSION TAG	UNP Q81T09
C	-4	HIS	-	EXPRESSION TAG	UNP Q81T09
C	-3	HIS	-	EXPRESSION TAG	UNP Q81T09
C	-2	HIS	-	EXPRESSION TAG	UNP Q81T09
C	-1	HIS	-	EXPRESSION TAG	UNP Q81T09
C	0	HIS	-	EXPRESSION TAG	UNP Q81T09
D	-9	MET	-	CLONING ARTIFACT	UNP Q81T09
D	-8	GLY	-	CLONING ARTIFACT	UNP Q81T09
D	-7	SER	-	CLONING ARTIFACT	UNP Q81T09
D	-6	SER	-	CLONING ARTIFACT	UNP Q81T09
D	-5	HIS	-	EXPRESSION TAG	UNP Q81T09
D	-4	HIS	-	EXPRESSION TAG	UNP Q81T09
D	-3	HIS	-	EXPRESSION TAG	UNP Q81T09
D	-2	HIS	-	EXPRESSION TAG	UNP Q81T09
D	-1	HIS	-	EXPRESSION TAG	UNP Q81T09
D	0	HIS	-	EXPRESSION TAG	UNP Q81T09
E	-9	MET	-	CLONING ARTIFACT	UNP Q81T09
E	-8	GLY	-	CLONING ARTIFACT	UNP Q81T09
E	-7	SER	-	CLONING ARTIFACT	UNP Q81T09
E	-6	SER	-	CLONING ARTIFACT	UNP Q81T09
E	-5	HIS	-	EXPRESSION TAG	UNP Q81T09
E	-4	HIS	-	EXPRESSION TAG	UNP Q81T09
E	-3	HIS	-	EXPRESSION TAG	UNP Q81T09
E	-2	HIS	-	EXPRESSION TAG	UNP Q81T09
E	-1	HIS	-	EXPRESSION TAG	UNP Q81T09
E	0	HIS	-	EXPRESSION TAG	UNP Q81T09
F	-9	MET	-	CLONING ARTIFACT	UNP Q81T09
F	-8	GLY	-	CLONING ARTIFACT	UNP Q81T09
F	-7	SER	-	CLONING ARTIFACT	UNP Q81T09
F	-6	SER	-	CLONING ARTIFACT	UNP Q81T09
F	-5	HIS	-	EXPRESSION TAG	UNP Q81T09
F	-4	HIS	-	EXPRESSION TAG	UNP Q81T09
F	-3	HIS	-	EXPRESSION TAG	UNP Q81T09
F	-2	HIS	-	EXPRESSION TAG	UNP Q81T09
F	-1	HIS	-	EXPRESSION TAG	UNP Q81T09

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	EXPRESSION TAG	UNP Q81T09

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

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

- Molecule 3 is water.

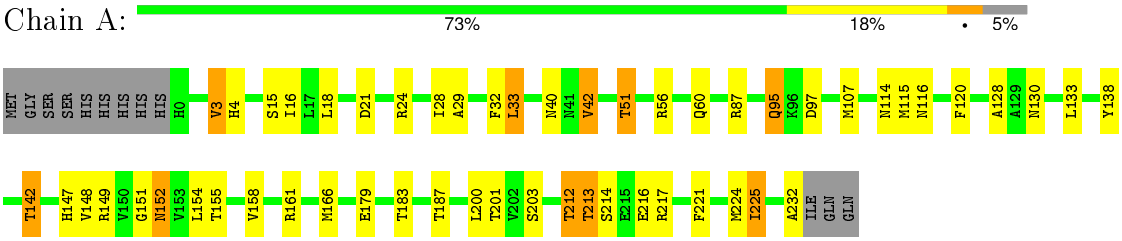
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	148	Total O 148 148	0	0
3	B	114	Total O 114 114	0	0
3	C	115	Total O 115 115	0	0
3	D	115	Total O 115 115	0	0
3	E	122	Total O 122 122	0	0
3	F	102	Total O 102 102	0	0

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.

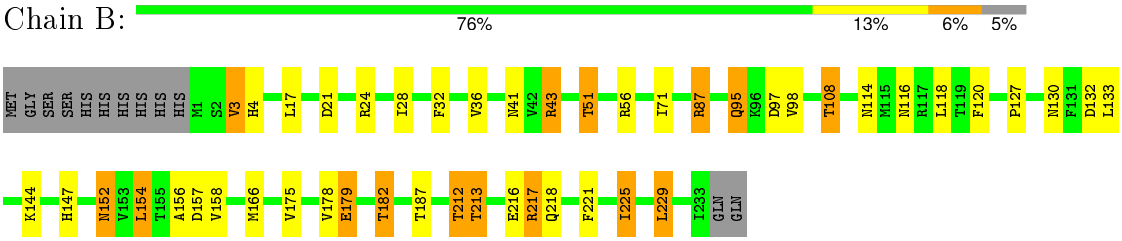
- Molecule 1: purine nucleoside phosphorylase

Chain A:



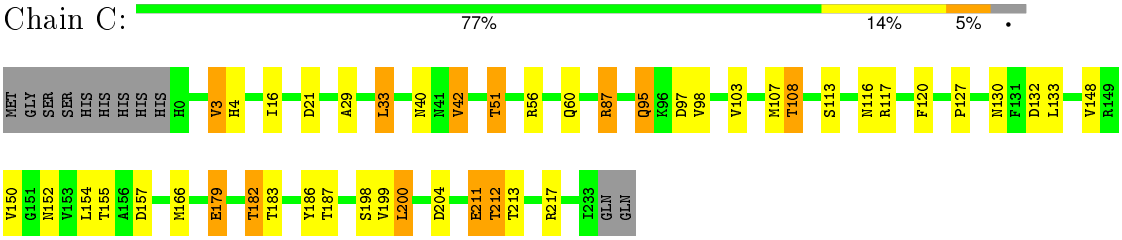
- Molecule 1: purine nucleoside phosphorylase

Chain B:



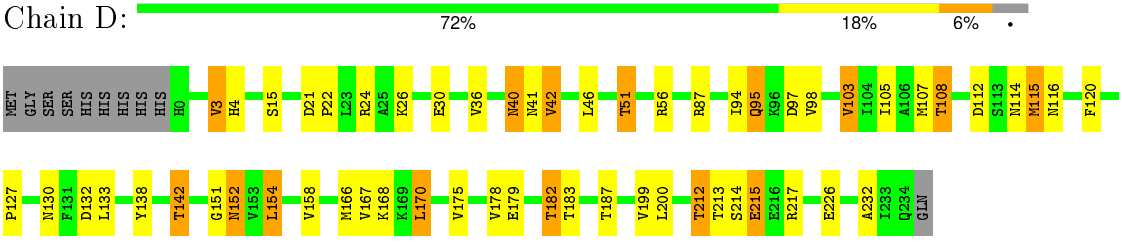
- Molecule 1: purine nucleoside phosphorylase

Chain C:



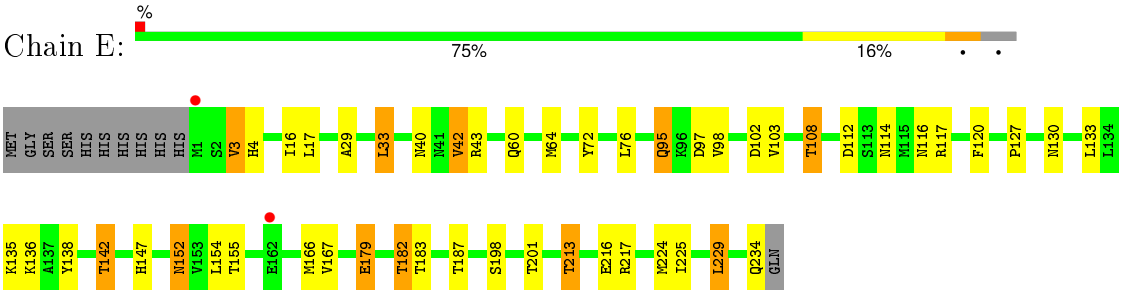
- Molecule 1: purine nucleoside phosphorylase

Chain D:



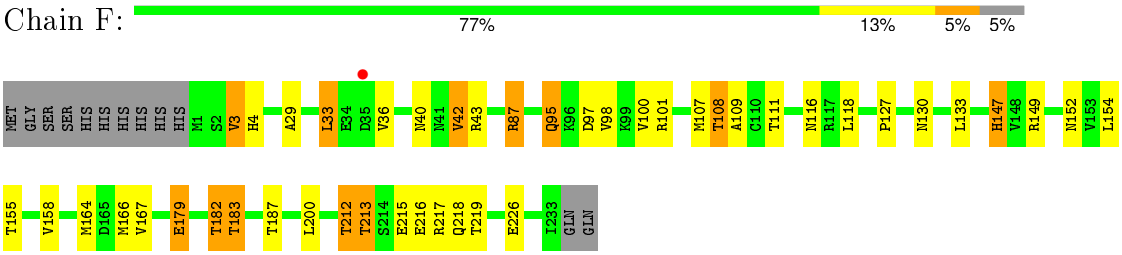
• Molecule 1: purine nucleoside phosphorylase

Chain E:



• Molecule 1: purine nucleoside phosphorylase

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.86Å 128.26Å 223.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.24 19.98 – 2.24	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-2.24) 90.9 (19.98-2.24)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.23Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.181 , 0.235 0.188 , 0.241	Depositor DCC
R_{free} test set	4065 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	22.5	Xtriage
Anisotropy	0.334	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 39.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 81160 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11450	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.90% 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: CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.63	0/1809	0.79	1/2447 (0.0%)
1	B	0.64	0/1806	0.77	2/2443 (0.1%)
1	C	0.63	0/1817	0.74	0/2458
1	D	0.67	0/1826	0.81	1/2470 (0.0%)
1	E	0.62	0/1815	0.78	1/2455 (0.0%)
1	F	0.64	0/1817	0.75	0/2457
All	All	0.64	0/10890	0.78	5/14730 (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	D	0	1

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	B	43	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	149	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	E	217	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	D	24	ARG	NE-CZ-NH2	-5.09	117.76	120.30
1	B	217	ARG	NE-CZ-NH1	5.04	122.82	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	40	ASN	Peptide

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	1782	0	1787	36	0
1	B	1780	0	1791	41	0
1	C	1790	0	1798	40	0
1	D	1799	0	1806	47	0
1	E	1789	0	1799	36	0
1	F	1788	0	1804	38	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	2	0
2	D	1	0	0	0	0
2	F	1	0	0	0	0
3	A	148	0	0	3	0
3	B	114	0	0	5	0
3	C	115	0	0	3	0
3	D	115	0	0	5	0
3	E	122	0	0	3	0
3	F	102	0	0	3	0
All	All	11450	0	10785	216	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 10.

All (216) 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:B:51:THR:HG22	1:B:56:ARG:HH11	1.41	0.85
1:A:158:VAL:HB	3:A:931:HOH:O	1.76	0.84
1:A:138:TYR:O	1:A:142:THR:HG23	1.77	0.84
1:E:138:TYR:O	1:E:142:THR:HG22	1.80	0.81
1:C:120:PHE:HA	1:E:166:MET:HE2	1.64	0.79
1:B:108:THR:HG22	1:B:127:PRO:O	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:THR:HG22	1:A:56:ARG:HH11	1.51	0.74
1:A:15:SER:HB3	1:A:232:ALA:HB1	1.71	0.73
1:D:213:THR:HG23	3:D:867:HOH:O	1.87	0.72
1:D:51:THR:HG22	1:D:56:ARG:HH11	1.54	0.71
1:D:138:TYR:O	1:D:142:THR:HG23	1.90	0.71
1:A:130:ASN:HD22	1:A:133:LEU:H	1.38	0.70
1:C:116:ASN:HD21	1:C:187:THR:HG21	1.56	0.70
1:B:108:THR:CG2	1:B:127:PRO:O	2.40	0.70
1:F:116:ASN:HD21	1:F:187:THR:HG21	1.57	0.69
1:E:40:ASN:OD1	1:E:42:VAL:HG13	1.92	0.69
1:B:51:THR:HG21	3:B:841:HOH:O	1.92	0.69
1:E:116:ASN:HD21	1:E:187:THR:HG21	1.56	0.68
1:C:51:THR:HG22	1:C:56:ARG:HH11	1.58	0.68
1:E:138:TYR:O	1:E:142:THR:CG2	2.42	0.68
1:D:41:ASN:HB3	1:D:46:LEU:HD23	1.76	0.68
1:A:116:ASN:HD21	1:A:187:THR:HG21	1.59	0.67
1:F:179:GLU:CD	1:F:182:THR:HG23	2.17	0.65
1:D:179:GLU:CD	1:D:182:THR:HG23	2.17	0.65
1:C:113:SER:O	2:C:806:CL:CL	2.52	0.65
1:D:130:ASN:HD22	1:D:133:LEU:H	1.43	0.64
1:A:28:ILE:HG23	1:A:225:ILE:HD13	1.80	0.64
1:B:87:ARG:HD2	3:B:870:HOH:O	1.99	0.63
1:F:130:ASN:HD22	1:F:133:LEU:H	1.46	0.62
1:B:212:THR:CG2	1:B:217:ARG:HD3	2.30	0.62
1:D:108:THR:HG22	1:D:127:PRO:O	1.99	0.62
1:B:225:ILE:HD12	1:B:229:LEU:HD22	1.81	0.62
1:A:51:THR:HG22	1:A:56:ARG:NH1	2.14	0.61
1:F:212:THR:HG22	1:F:217:ARG:HH11	1.65	0.61
1:D:87:ARG:HD2	3:D:892:HOH:O	2.01	0.60
1:E:213:THR:HG22	1:E:216:GLU:H	1.66	0.60
1:F:108:THR:CG2	1:F:127:PRO:O	2.50	0.60
1:A:40:ASN:OD1	1:A:42:VAL:HG13	2.02	0.60
1:B:28:ILE:HG23	1:B:225:ILE:HD13	1.83	0.60
1:F:179:GLU:OE1	1:F:182:THR:HG23	2.02	0.59
1:C:179:GLU:CD	1:C:182:THR:HG23	2.22	0.59
1:C:213:THR:HG21	3:C:854:HOH:O	2.02	0.59
1:F:40:ASN:OD1	1:F:42:VAL:CG1	2.50	0.59
1:F:213:THR:HG21	3:F:851:HOH:O	2.01	0.59
1:B:95:GLN:HE21	1:B:98:VAL:HG23	1.68	0.59
1:B:166:MET:HE1	1:D:120:PHE:HD2	1.68	0.59
1:F:213:THR:HG22	1:F:216:GLU:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:111:THR:HB	1:F:183:THR:HG21	1.85	0.58
1:C:95:GLN:HE21	1:C:98:VAL:HG23	1.69	0.58
1:E:16:ILE:HD11	1:E:60:GLN:HB2	1.84	0.58
1:A:114:ASN:HB2	1:D:114:ASN:HB2	1.86	0.57
1:F:87[A]:ARG:NH1	1:F:179:GLU:OE1	2.38	0.57
1:A:130:ASN:ND2	1:A:133:LEU:H	2.03	0.57
1:E:155:THR:HG21	1:E:183:THR:HG22	1.85	0.57
1:F:108:THR:HG22	1:F:127:PRO:O	2.04	0.57
1:D:108:THR:CG2	1:D:127:PRO:O	2.53	0.57
1:F:95:GLN:HE21	1:F:98:VAL:HG23	1.69	0.57
1:C:179:GLU:OE1	1:C:182:THR:HG23	2.05	0.57
1:B:108:THR:HG21	1:D:108:THR:HG21	1.86	0.57
1:F:40:ASN:OD1	1:F:42:VAL:HG12	2.05	0.57
1:B:71:ILE:HD13	1:E:64:MET:HE1	1.86	0.56
1:E:136:LYS:NZ	1:E:234:GLN:OE1	2.38	0.56
1:C:212:THR:CG2	1:C:217:ARG:HD3	2.35	0.56
1:D:179:GLU:OE1	1:D:182:THR:HG23	2.05	0.56
1:A:120:PHE:HA	1:F:166:MET:HE1	1.88	0.56
1:F:155:THR:CB	1:F:183:THR:HG23	2.36	0.55
1:B:120:PHE:CD2	1:D:170:LEU:HD13	2.41	0.55
1:C:166:MET:CE	1:E:120:PHE:HD2	2.19	0.55
1:E:142:THR:HB	3:E:357:HOH:O	2.07	0.55
1:B:43:ARG:NH2	3:B:888:HOH:O	2.38	0.55
1:C:166:MET:HE1	1:E:120:PHE:HD2	1.72	0.55
1:B:166:MET:HE1	1:D:120:PHE:CD2	2.41	0.55
1:A:95:GLN:NE2	1:A:97:ASP:H	2.05	0.55
1:B:114:ASN:HB2	1:E:114:ASN:HB2	1.88	0.55
1:A:155:THR:HG21	1:A:183:THR:HG22	1.90	0.54
1:B:120:PHE:HD2	1:D:166:MET:HE1	1.73	0.54
1:E:179:GLU:CD	1:E:182:THR:HG23	2.28	0.53
1:C:108:THR:HG21	1:E:108:THR:HG21	1.89	0.53
1:A:29:ALA:HA	1:A:33:LEU:HD22	1.89	0.53
1:F:218:GLN:HG3	3:F:886:HOH:O	2.08	0.53
1:A:212:THR:CG2	1:A:217:ARG:HH11	2.21	0.53
1:E:29:ALA:HA	1:E:33:LEU:HD22	1.90	0.53
1:B:130:ASN:HD22	1:B:133:LEU:H	1.54	0.53
1:B:179:GLU:CD	1:B:182:THR:HG23	2.29	0.53
1:E:17:LEU:HD11	1:E:229:LEU:HD13	1.91	0.53
1:B:166:MET:CE	1:D:120:PHE:HD2	2.22	0.53
1:D:213:THR:HG21	3:D:915:HOH:O	2.09	0.52
1:A:16:ILE:HD11	1:A:60:GLN:HB2	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:94:ILE:HD11	1:D:175:VAL:HG22	1.90	0.52
1:F:147:HIS:HD2	3:F:827:HOH:O	1.93	0.52
1:B:218:GLN:HG3	3:B:903:HOH:O	2.10	0.52
1:D:51:THR:HG22	1:D:56:ARG:NH1	2.24	0.52
1:F:109:ALA:CB	1:F:183:THR:HG22	2.40	0.52
1:A:213:THR:HG22	1:A:216:GLU:H	1.74	0.52
1:C:95:GLN:HE22	1:C:97:ASP:HB2	1.74	0.52
1:E:3:VAL:HG22	1:E:4:HIS:CE1	2.45	0.52
1:D:212:THR:CG2	1:D:217:ARG:HH11	2.23	0.52
1:B:120:PHE:HD2	1:D:166:MET:CE	2.23	0.51
1:D:212:THR:HG23	1:D:217:ARG:HG3	1.92	0.51
1:D:15:SER:HB3	1:D:232:ALA:HB1	1.93	0.51
1:F:29:ALA:HA	1:F:33:LEU:HD22	1.92	0.51
1:C:3:VAL:HG22	1:C:4:HIS:CE1	2.45	0.51
1:C:40:ASN:OD1	1:C:42:VAL:HG13	2.10	0.51
1:C:166:MET:HE1	1:E:120:PHE:CD2	2.46	0.51
1:D:3:VAL:HG22	1:D:4:HIS:CE1	2.47	0.50
1:B:51:THR:HG22	1:B:56:ARG:NH1	2.19	0.50
1:D:95:GLN:HE21	1:D:98:VAL:HG23	1.75	0.50
1:C:108:THR:CG2	1:C:127:PRO:O	2.59	0.50
1:B:130:ASN:ND2	1:B:133:LEU:H	2.09	0.50
1:B:120:PHE:CD2	1:D:166:MET:HE1	2.47	0.50
1:A:95:GLN:HE22	1:A:97:ASP:H	1.60	0.50
1:C:130:ASN:HD22	1:C:133:LEU:H	1.59	0.50
1:D:94:ILE:HD11	1:D:175:VAL:CG2	2.42	0.50
1:D:105:ILE:HG12	1:D:199:VAL:HG22	1.94	0.50
1:D:116:ASN:HD21	1:D:187:THR:HG21	1.76	0.50
1:B:116:ASN:HD21	1:B:187:THR:HG21	1.77	0.50
1:D:26:LYS:NZ	1:D:30:GLU:OE2	2.36	0.49
1:E:72:TYR:O	1:E:76:LEU:HG	2.12	0.49
1:A:107:MET:CE	1:A:151:GLY:HA2	2.43	0.49
1:E:179:GLU:OE1	1:E:182:THR:HG23	2.12	0.49
1:A:147:HIS:HD2	3:A:843:HOH:O	1.94	0.49
1:F:95:GLN:NE2	1:F:97:ASP:H	2.10	0.49
1:E:95:GLN:HE21	1:E:98:VAL:HG23	1.78	0.48
1:C:127:PRO:HB2	1:C:186:TYR:HB3	1.94	0.48
1:D:40:ASN:OD1	1:D:42:VAL:HG13	2.14	0.48
1:D:212:THR:HG22	1:D:217:ARG:HH11	1.78	0.48
1:E:130:ASN:HD22	1:E:133:LEU:H	1.62	0.48
1:F:130:ASN:ND2	1:F:133:LEU:H	2.12	0.48
1:B:130:ASN:HD21	1:B:132:ASP:HB3	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:ALA:HA	1:C:33:LEU:HD22	1.95	0.48
1:E:152:ASN:HD22	1:E:152:ASN:H	1.61	0.48
1:A:21:ASP:HB3	1:A:24:ARG:HD3	1.97	0.47
1:B:225:ILE:CD1	1:B:229:LEU:HD22	2.44	0.47
1:E:182:THR:HB	1:E:198:SER:OG	2.13	0.47
1:F:212:THR:CG2	1:F:217:ARG:HD3	2.45	0.47
1:F:108:THR:HG23	1:F:127:PRO:O	2.15	0.47
1:D:170:LEU:O	1:D:175:VAL:HG13	2.14	0.47
1:E:95:GLN:NE2	1:E:97:ASP:H	2.13	0.47
1:A:128:ALA:HB1	1:F:107:MET:HE3	1.96	0.47
1:B:3:VAL:HG22	1:B:4:HIS:CE1	2.50	0.46
1:C:21:ASP:OD1	1:F:43:ARG:HA	2.15	0.46
1:B:32:PHE:CE2	1:B:225:ILE:HG12	2.50	0.46
1:B:17:LEU:HD11	1:B:229:LEU:HD13	1.96	0.46
1:B:147:HIS:HD2	3:B:815:HOH:O	1.99	0.46
1:F:95:GLN:HE22	1:F:97:ASP:HB2	1.81	0.46
1:C:212:THR:CG2	1:C:217:ARG:HH11	2.29	0.46
1:D:213:THR:HG22	1:D:215:GLU:N	2.31	0.46
1:D:130:ASN:ND2	1:D:133:LEU:H	2.11	0.46
1:C:213:THR:HG23	3:C:842:HOH:O	2.16	0.45
1:A:120:PHE:HD2	1:F:166:MET:HE1	1.81	0.45
1:E:108:THR:CG2	1:E:127:PRO:O	2.64	0.45
1:A:203:SER:O	1:A:212:THR:HG22	2.17	0.45
1:B:21:ASP:OD1	1:E:43:ARG:HA	2.16	0.45
1:B:154:LEU:HD13	1:B:156:ALA:HB2	1.99	0.45
1:B:221:PHE:O	1:B:225:ILE:HG23	2.16	0.45
1:F:109:ALA:HB3	1:F:183:THR:HG22	1.97	0.45
1:F:100:VAL:O	1:F:101:ARG:HB2	2.17	0.45
1:B:108:THR:HG23	1:B:127:PRO:O	2.16	0.45
1:C:213:THR:CG2	3:C:842:HOH:O	2.65	0.45
1:D:132:ASP:HB3	3:D:912:HOH:O	2.16	0.45
1:C:130:ASN:HD21	1:C:132:ASP:HB3	1.82	0.44
1:C:107:MET:HE2	1:C:150:VAL:HG12	1.98	0.44
1:C:179:GLU:OE1	1:C:182:THR:CG2	2.66	0.44
1:A:212:THR:HG22	1:A:217:ARG:HH11	1.81	0.44
1:A:138:TYR:O	1:A:142:THR:CG2	2.59	0.44
1:C:51:THR:HG22	1:C:56:ARG:NH1	2.29	0.44
1:C:108:THR:HG23	1:C:127:PRO:O	2.16	0.44
1:D:95:GLN:HE22	1:D:97:ASP:HB2	1.83	0.44
1:B:212:THR:HG21	1:B:217:ARG:HD3	2.00	0.44
1:F:29:ALA:O	1:F:33:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:MET:HE1	1:D:183:THR:HG23	1.99	0.44
1:D:152:ASN:ND2	1:D:175:VAL:HA	2.32	0.44
1:D:103:VAL:HA	1:D:200:LEU:O	2.19	0.43
1:C:117:ARG:HG3	2:C:806:CL:CL	2.55	0.43
1:C:212:THR:HG21	1:C:217:ARG:HD3	1.99	0.43
1:A:212:THR:CG2	1:A:217:ARG:HD3	2.49	0.43
1:E:130:ASN:ND2	1:E:133:LEU:H	2.17	0.43
1:C:155:THR:HG21	1:C:183:THR:HG22	2.01	0.43
1:E:201:THR:OG1	1:E:224:MET:SD	2.77	0.43
1:F:179:GLU:OE1	1:F:182:THR:CG2	2.66	0.43
1:C:95:GLN:HB3	1:C:98:VAL:HG23	2.01	0.42
1:E:102:ASP:HA	1:E:147:HIS:HB2	2.00	0.42
1:F:3:VAL:HG22	1:F:4:HIS:CE1	2.54	0.42
1:D:107:MET:CE	1:D:151:GLY:HA2	2.49	0.42
1:D:226:GLU:HB2	3:D:903:HOH:O	2.20	0.42
1:B:152:ASN:ND2	1:B:175:VAL:HA	2.35	0.42
1:D:179:GLU:OE1	1:D:182:THR:CG2	2.67	0.42
1:A:18:LEU:O	1:A:87:ARG:HD2	2.19	0.42
1:A:152:ASN:HD22	1:A:152:ASN:H	1.67	0.42
1:D:21:ASP:HA	1:D:22:PRO:HD2	1.86	0.42
1:B:95:GLN:HE22	1:B:97:ASP:HB2	1.85	0.41
1:C:108:THR:HG22	1:C:127:PRO:O	2.20	0.41
1:B:152:ASN:HD22	1:B:152:ASN:H	1.68	0.41
1:B:213:THR:HG22	1:B:216:GLU:H	1.86	0.41
1:A:161:ARG:CZ	3:A:931:HOH:O	2.68	0.41
1:C:179:GLU:HG2	1:C:200:LEU:HD21	2.02	0.41
1:D:107:MET:HE3	1:D:151:GLY:HA2	2.03	0.41
1:C:16:ILE:HD11	1:C:60:GLN:HB2	2.03	0.41
1:E:64:MET:CE	3:E:291:HOH:O	2.69	0.41
1:C:204:ASP:HB3	1:C:211:GLU:HA	2.03	0.41
1:F:155:THR:HB	1:F:183:THR:HG23	2.03	0.41
1:C:116:ASN:HD21	1:C:187:THR:CG2	2.30	0.41
1:C:182:THR:HB	1:C:198:SER:OG	2.21	0.41
1:E:64:MET:HE2	3:E:291:HOH:O	2.21	0.41
1:F:109:ALA:HB1	1:F:183:THR:HG22	2.03	0.40
1:E:225:ILE:HG22	1:E:229:LEU:HD22	2.03	0.40
1:A:3:VAL:HG22	1:A:4:HIS:CE1	2.57	0.40
1:A:201:THR:OG1	1:A:224:MET:SD	2.80	0.40
1:F:164:MET:CE	1:F:167:VAL:HG21	2.51	0.40
1:A:221:PHE:O	1:A:225:ILE:HG23	2.21	0.40
1:F:212:THR:CG2	1:F:217:ARG:HH11	2.32	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:ARG:NH1	1:C:179:GLU:OE1	2.55	0.40
1:A:32:PHE:CE2	1:A:225:ILE:HG12	2.57	0.40
1:A:120:PHE:CD2	1:F:166:MET:HE1	2.57	0.40
1:E:108:THR:HG22	1:E:127:PRO:O	2.22	0.40
1:D:154:LEU:HD13	1:D:178:VAL:HG23	2.03	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	231/245 (94%)	231 (100%)	0	0	100	100
1	B	231/245 (94%)	228 (99%)	3 (1%)	0	100	100
1	C	232/245 (95%)	229 (99%)	3 (1%)	0	100	100
1	D	233/245 (95%)	231 (99%)	2 (1%)	0	100	100
1	E	232/245 (95%)	227 (98%)	5 (2%)	0	100	100
1	F	232/245 (95%)	230 (99%)	2 (1%)	0	100	100
All	All	1391/1470 (95%)	1376 (99%)	15 (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	192/203 (95%)	175 (91%)	17 (9%)	12 8
1	B	192/203 (95%)	171 (89%)	21 (11%)	8 5
1	C	193/203 (95%)	175 (91%)	18 (9%)	11 7
1	D	194/203 (96%)	174 (90%)	20 (10%)	9 5
1	E	193/203 (95%)	176 (91%)	17 (9%)	12 9
1	F	193/203 (95%)	170 (88%)	23 (12%)	6 3
All	All	1157/1218 (95%)	1041 (90%)	116 (10%)	10 6

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	33	LEU
1	A	42	VAL
1	A	51	THR
1	A	95	GLN
1	A	115	MET
1	A	142	THR
1	A	148	VAL
1	A	152	ASN
1	A	154	LEU
1	A	166	MET
1	A	179	GLU
1	A	200	LEU
1	A	212	THR
1	A	213	THR
1	A	214	SER
1	A	225	ILE
1	B	3	VAL
1	B	24	ARG
1	B	36	VAL
1	B	41	ASN
1	B	51	THR
1	B	87	ARG
1	B	95	GLN
1	B	108	THR
1	B	118	LEU
1	B	144	LYS
1	B	152	ASN
1	B	154	LEU
1	B	157	ASP

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Mol	Chain	Res	Type
1	B	158	VAL
1	B	178	VAL
1	B	179	GLU
1	B	182	THR
1	B	212	THR
1	B	213	THR
1	B	225	ILE
1	B	229	LEU
1	C	3	VAL
1	C	33	LEU
1	C	42	VAL
1	C	51	THR
1	C	87	ARG
1	C	95	GLN
1	C	103	VAL
1	C	108	THR
1	C	148	VAL
1	C	152	ASN
1	C	154	LEU
1	C	157	ASP
1	C	179	GLU
1	C	182	THR
1	C	199	VAL
1	C	200	LEU
1	C	211	GLU
1	C	212	THR
1	D	3	VAL
1	D	36	VAL
1	D	42	VAL
1	D	51	THR
1	D	95	GLN
1	D	103	VAL
1	D	108	THR
1	D	112	ASP
1	D	115	MET
1	D	142	THR
1	D	152	ASN
1	D	154	LEU
1	D	158	VAL
1	D	167	VAL
1	D	168	LYS
1	D	170	LEU

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Mol	Chain	Res	Type
1	D	182	THR
1	D	212	THR
1	D	214	SER
1	D	215	GLU
1	E	3	VAL
1	E	33	LEU
1	E	42	VAL
1	E	95	GLN
1	E	103	VAL
1	E	108	THR
1	E	112	ASP
1	E	117	ARG
1	E	135	LYS
1	E	142	THR
1	E	152	ASN
1	E	154	LEU
1	E	167	VAL
1	E	179	GLU
1	E	182	THR
1	E	213	THR
1	E	229	LEU
1	F	3	VAL
1	F	33	LEU
1	F	36	VAL
1	F	42	VAL
1	F	87[A]	ARG
1	F	87[B]	ARG
1	F	95	GLN
1	F	108	THR
1	F	118	LEU
1	F	147	HIS
1	F	149	ARG
1	F	152	ASN
1	F	154	LEU
1	F	158	VAL
1	F	179	GLU
1	F	182	THR
1	F	183	THR
1	F	200	LEU
1	F	212	THR
1	F	213	THR
1	F	215	GLU

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Mol	Chain	Res	Type
1	F	219	THR
1	F	226	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	95	GLN
1	A	116	ASN
1	A	130	ASN
1	A	147	HIS
1	A	152	ASN
1	A	195	ASN
1	B	95	GLN
1	B	116	ASN
1	B	130	ASN
1	B	147	HIS
1	B	152	ASN
1	B	195	ASN
1	C	95	GLN
1	C	116	ASN
1	C	130	ASN
1	C	147	HIS
1	C	152	ASN
1	C	195	ASN
1	D	95	GLN
1	D	116	ASN
1	D	130	ASN
1	D	152	ASN
1	D	195	ASN
1	E	9	GLN
1	E	95	GLN
1	E	116	ASN
1	E	130	ASN
1	E	147	HIS
1	E	152	ASN
1	E	195	ASN
1	F	74	ASN
1	F	95	GLN
1	F	116	ASN
1	F	130	ASN
1	F	147	HIS

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Mol	Chain	Res	Type
1	F	152	ASN
1	F	195	ASN

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 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	233/245 (95%)	-0.50	0	100	100	15, 21, 29, 35	0
1	B	233/245 (95%)	-0.49	0	100	100	16, 21, 29, 35	0
1	C	234/245 (95%)	-0.48	0	100	100	14, 21, 28, 35	0
1	D	235/245 (95%)	-0.44	0	100	100	13, 21, 31, 40	0
1	E	234/245 (95%)	-0.36	2 (0%)	85	86	15, 22, 32, 42	0
1	F	233/245 (95%)	-0.39	1 (0%)	93	94	16, 22, 33, 40	0
All	All	1402/1470 (95%)	-0.45	3 (0%)	95	96	13, 21, 31, 42	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1	MET	3.6
1	E	162	GLU	2.9
1	F	35	ASP	2.4

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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	CL	C	806	1/1	0.99	0.22	4.82	24,24,24,24	0
2	CL	B	801	1/1	0.99	0.07	-0.95	23,23,23,23	0
2	CL	D	804	1/1	1.00	0.09	-1.14	16,16,16,16	0
2	CL	F	803	1/1	1.00	0.09	-1.25	17,17,17,17	0
2	CL	A	805	1/1	0.98	0.06	-1.57	26,26,26,26	0
2	CL	C	802	1/1	0.99	0.06	-2.60	17,17,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.