Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:39 AM GMT

PDB ID	:	2B99
Title	:	Crystal Structure of an archaeal pentameric riboflavin synthase Complex with a Substrate analog inhibitor
Authors	:	Ramsperger, A.; Augustin, M.; Schott, A.K.; Gerhardt, S.; Krojer, T.; Eisenreich, W.; Illarionov, B.; Cushman, M.; Bacher, A.; Huber, R.; Fischer, M.
Deposited on	:	2005-10-11
Resolution	:	2.22 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:

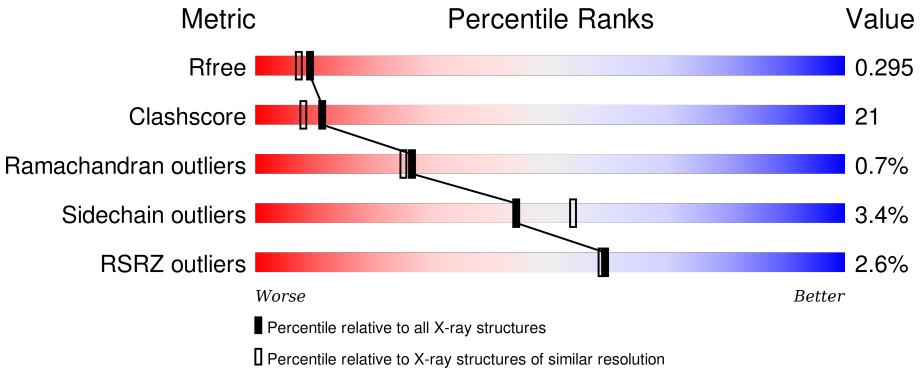
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.22 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	4405 (2.24-2.20)
Clashscore	102246	5146 (2.24-2.20)
Ramachandran outliers	100387	5065 (2.24-2.20)
Sidechain outliers	100360	5066 (2.24-2.20)
RSRZ outliers	91569	4414 (2.24-2.20)

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	156	4% 67% 22% • 6%
1	B	156	4% 63% 26% • • 8%
1	C	156	% 66% 27% • •
1	D	156	3% 62% 26% • 10%
1	E	156	% 69% 26% • •

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	RDL	A	1208	-	-	-	X
2	RDL	B	1209	-	-	-	X
2	RDL	C	1204	-	-	-	X
2	RDL	D	1203	-	-	-	X

2 Entry composition

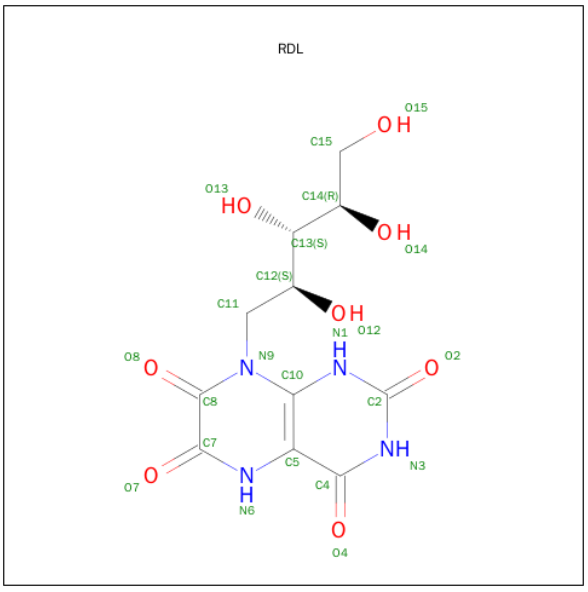
There are 3 unique types of molecules in this entry. The entry contains 6187 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Riboflavin synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	146	Total	C	N	O	S	65	0	0
			1145	730	197	209	9			
1	B	143	Total	C	N	O	S	67	0	0
			1121	717	190	205	9			
1	C	152	Total	C	N	O	S	50	0	0
			1189	758	203	219	9			
1	D	141	Total	C	N	O	S	51	0	0
			1106	707	188	202	9			
1	E	152	Total	C	N	O	S	53	0	0
			1189	758	203	219	9			

- Molecule 2 is 6,7-DIOXO-5H-8-RIBITYLAMINOLUMAZINE (three-letter code: RDL) (formula: $C_{11}H_{14}N_4O_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			23	11	4	8		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	E	1	Total	C	N	O	0	0
			23	11	4	8		
2	D	1	Total	C	N	O	0	0
			23	11	4	8		
2	C	1	Total	C	N	O	0	0
			23	11	4	8		
2	A	1	Total	C	N	O	0	0
			23	11	4	8		
2	B	1	Total	C	N	O	23	0
			23	11	4	8		
2	E	1	Total	C	N	O	0	0
			23	11	4	8		
2	A	1	Total	C	N	O	0	0
			23	11	4	8		
2	B	1	Total	C	N	O	0	0
			23	11	4	8		
2	B	1	Total	C	N	O	0	0
			23	11	4	8		

- Molecule 3 is water.

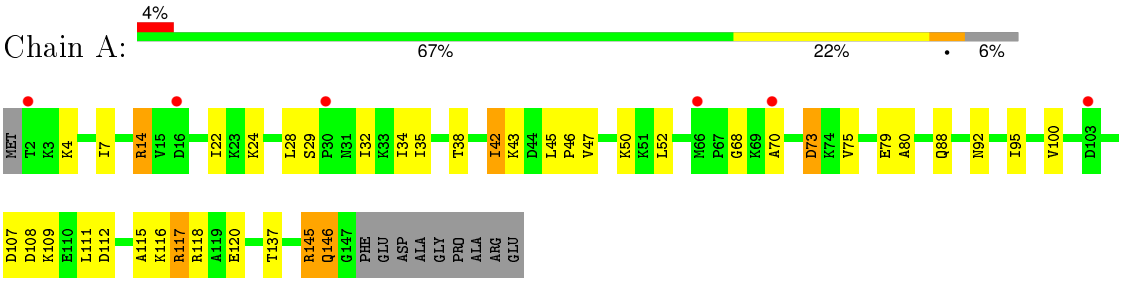
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total	O	0	0
			39	39		
3	B	44	Total	O	0	0
			44	44		
3	C	50	Total	O	0	0
			50	50		
3	D	33	Total	O	0	0
			33	33		
3	E	41	Total	O	0	0
			41	41		

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.

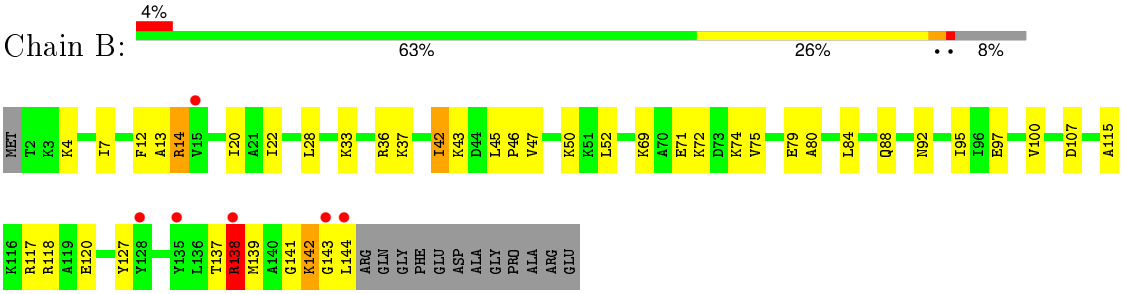
- Molecule 1: Riboflavin synthase

Chain A:



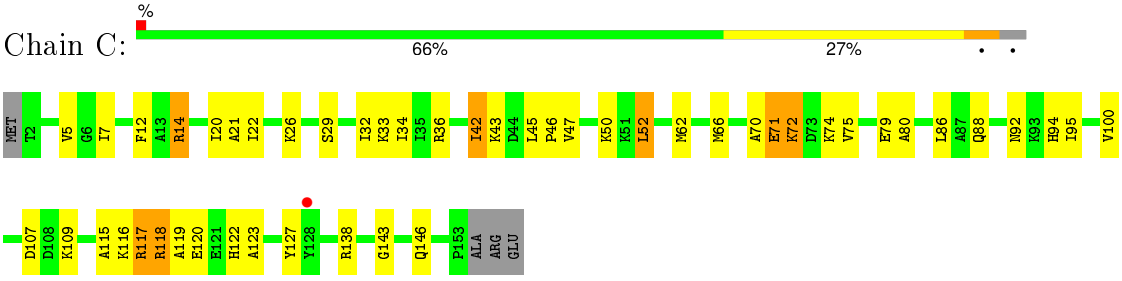
- Molecule 1: Riboflavin synthase

Chain B:



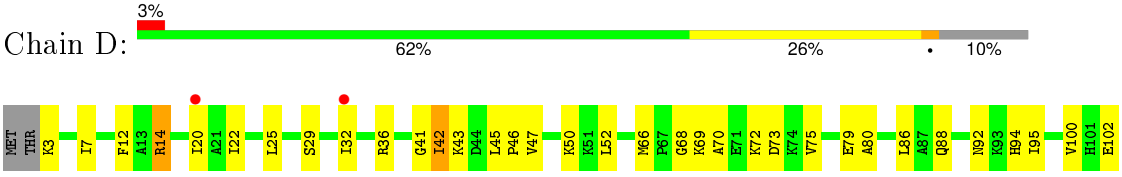
- Molecule 1: Riboflavin synthase

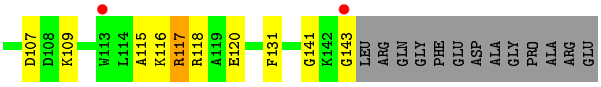
Chain C:



- Molecule 1: Riboflavin synthase

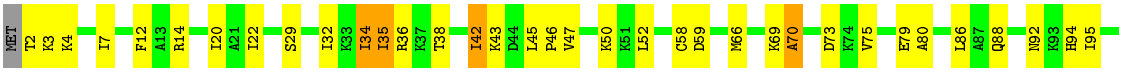
Chain D:

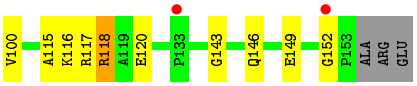




• Molecule 1: Riboflavin synthase

Chain E:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	41.94Å 72.91Å 72.78Å 68.50° 74.39° 74.53°	Depositor
Resolution (Å)	19.92 – 2.22 19.92 – 2.22	Depositor EDS
% Data completeness (in resolution range)	93.0 (19.92-2.22) 82.6 (19.92-2.22)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 2.21Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.258 , 0.296 0.259 , 0.295	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	28.6	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 23.2	EDS
Estimated twinning fraction	0.077 for h,h-k,h-l 0.208 for -h,-l,-k 0.075 for -h,-h+l,-h+k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 36722 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6187	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.96% 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: RDL

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	0.38	0/1161	0.97	8/1556 (0.5%)
1	B	0.37	0/1137	1.22	11/1525 (0.7%)
1	C	0.38	0/1207	0.92	9/1619 (0.6%)
1	D	0.36	0/1122	0.96	7/1504 (0.5%)
1	E	0.37	0/1207	0.85	6/1619 (0.4%)
All	All	0.37	0/5834	0.99	41/7823 (0.5%)

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	138	ARG	NE-CZ-NH1	18.05	129.33	120.30
1	B	138	ARG	NE-CZ-NH2	-17.82	111.39	120.30
1	B	14	ARG	NE-CZ-NH2	-15.38	112.61	120.30
1	C	14	ARG	NE-CZ-NH2	-14.28	113.16	120.30
1	B	14	ARG	NE-CZ-NH1	14.25	127.42	120.30
1	D	117	ARG	NE-CZ-NH1	-14.12	113.24	120.30
1	D	117	ARG	NE-CZ-NH2	13.25	126.93	120.30
1	A	117	ARG	NE-CZ-NH1	-13.00	113.80	120.30
1	A	118	ARG	NE-CZ-NH1	-12.70	113.95	120.30
1	B	118	ARG	NE-CZ-NH1	-12.65	113.97	120.30
1	A	117	ARG	NE-CZ-NH2	12.38	126.49	120.30
1	A	118	ARG	NE-CZ-NH2	12.31	126.46	120.30
1	B	118	ARG	NE-CZ-NH2	12.28	126.44	120.30
1	C	14	ARG	NE-CZ-NH1	12.27	126.44	120.30
1	D	14	ARG	NE-CZ-NH1	-11.29	114.66	120.30
1	D	14	ARG	NE-CZ-NH2	10.33	125.47	120.30
1	E	14	ARG	NE-CZ-NH1	-9.94	115.33	120.30
1	B	117	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	C	118	ARG	NE-CZ-NH2	-9.04	115.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	117	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	E	118	ARG	NE-CZ-NH2	-9.00	115.80	120.30
1	A	14	ARG	NE-CZ-NH1	-8.97	115.82	120.30
1	E	14	ARG	NE-CZ-NH2	8.95	124.77	120.30
1	E	117	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	D	118	ARG	NE-CZ-NH2	-8.83	115.89	120.30
1	E	118	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	E	117	ARG	NE-CZ-NH2	-8.75	115.92	120.30
1	C	118	ARG	NE-CZ-NH1	8.57	124.59	120.30
1	D	118	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	A	14	ARG	NE-CZ-NH2	8.07	124.34	120.30
1	B	138	ARG	CD-NE-CZ	7.92	134.69	123.60
1	C	117	ARG	NE-CZ-NH1	7.85	124.22	120.30
1	C	117	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	C	117	ARG	CB-CG-CD	7.20	130.32	111.60
1	B	14	ARG	CD-NE-CZ	6.58	132.81	123.60
1	C	14	ARG	CD-NE-CZ	6.53	132.74	123.60
1	A	117	ARG	CD-NE-CZ	5.96	131.95	123.60
1	D	117	ARG	CD-NE-CZ	5.77	131.68	123.60
1	A	118	ARG	CD-NE-CZ	5.68	131.55	123.60
1	B	118	ARG	CD-NE-CZ	5.59	131.43	123.60
1	C	117	ARG	CG-CD-NE	5.10	122.50	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1145	0	1204	51	0
1	B	1121	0	1180	53	0
1	C	1189	0	1238	60	0
1	D	1106	0	1162	52	0
1	E	1189	0	1238	56	0
2	A	46	0	28	1	0
2	B	69	0	42	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	46	0	28	2	0
2	D	23	0	14	6	0
2	E	46	0	28	2	0
3	A	39	0	0	3	0
3	B	44	0	0	5	0
3	C	50	0	0	10	0
3	D	33	0	0	5	0
3	E	41	0	0	2	0
All	All	6187	0	6162	233	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 21.

All (233) 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:47:VAL:HG21	1:E:88:GLN:HB3	1.23	1.16
1:A:47:VAL:HG21	1:B:88:GLN:HB3	1.25	1.15
1:B:47:VAL:HG21	1:D:88:GLN:HB3	1.25	1.14
1:A:88:GLN:HB3	1:E:47:VAL:HG21	1.29	1.13
1:C:88:GLN:HB3	1:D:47:VAL:HG21	1.26	1.10
1:E:35:ILE:HD11	1:E:58:CYS:SG	2.00	1.02
1:A:146:GLN:HE21	1:A:146:GLN:HA	1.26	1.01
2:D:1203:RDL:H121	3:D:1209:HOH:O	1.63	0.97
1:B:142:LYS:HG2	1:B:143:GLY:H	1.29	0.94
1:A:29:SER:O	1:A:32:ILE:HG13	1.72	0.90
1:B:47:VAL:CG2	1:D:88:GLN:HB3	2.01	0.89
1:C:123:ALA:HB2	3:C:1248:HOH:O	1.70	0.89
1:A:47:VAL:CG2	1:B:88:GLN:HB3	2.04	0.88
1:C:47:VAL:CG2	1:E:88:GLN:HB3	2.02	0.88
1:C:88:GLN:HB3	1:D:47:VAL:CG2	2.06	0.86
1:B:143:GLY:O	1:B:144:LEU:HB2	1.76	0.86
1:A:88:GLN:HB3	1:E:47:VAL:CG2	2.05	0.86
1:B:42:ILE:HG23	1:B:80:ALA:HB2	1.58	0.86
1:B:142:LYS:HG2	1:B:143:GLY:N	1.90	0.85
1:C:42:ILE:HG23	1:C:80:ALA:HB2	1.59	0.83
1:E:42:ILE:HG23	1:E:80:ALA:HB2	1.61	0.83
1:A:42:ILE:HG23	1:A:80:ALA:HB2	1.61	0.81
1:D:42:ILE:HG23	1:D:80:ALA:HB2	1.62	0.81
1:D:75:VAL:O	1:D:79:GLU:HG3	1.81	0.80
1:C:62:MET:HE1	3:C:1248:HOH:O	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:SER:O	1:D:32:ILE:HG12	1.82	0.80
1:B:142:LYS:CG	1:B:143:GLY:H	1.93	0.80
1:E:75:VAL:O	1:E:79:GLU:HG3	1.82	0.78
1:A:75:VAL:O	1:A:79:GLU:HG3	1.84	0.78
1:E:47:VAL:HG23	3:E:1211:HOH:O	1.82	0.78
1:C:75:VAL:O	1:C:79:GLU:HG3	1.84	0.77
1:B:75:VAL:O	1:B:79:GLU:HG3	1.83	0.77
1:A:47:VAL:HG23	3:A:1209:HOH:O	1.84	0.76
1:C:47:VAL:HG21	1:E:88:GLN:CB	2.12	0.76
1:D:41:GLY:HA3	2:D:1203:RDL:O12	1.86	0.75
1:C:88:GLN:CB	1:D:47:VAL:HG21	2.14	0.73
1:E:7:ILE:HD12	1:E:34:ILE:HD11	1.69	0.73
1:A:47:VAL:HG21	1:B:88:GLN:CB	2.13	0.72
1:D:47:VAL:HG23	3:D:1207:HOH:O	1.89	0.72
1:A:32:ILE:O	1:A:32:ILE:HD12	1.88	0.72
1:B:47:VAL:HG21	1:D:88:GLN:CB	2.15	0.71
1:A:22:ILE:HG23	1:A:34:ILE:CD1	2.22	0.70
1:C:47:VAL:HG23	3:C:1208:HOH:O	1.92	0.70
1:A:29:SER:OG	1:A:32:ILE:HG23	1.92	0.70
1:B:71:GLU:HA	1:B:74:LYS:HE2	1.73	0.69
1:C:119:ALA:O	3:C:1248:HOH:O	2.11	0.69
1:A:88:GLN:CB	1:E:47:VAL:HG21	2.18	0.67
1:E:7:ILE:HD12	1:E:34:ILE:CD1	2.25	0.67
1:C:42:ILE:HG23	1:C:80:ALA:CB	2.27	0.64
1:A:70:ALA:HB3	1:A:73:ASP:OD1	1.97	0.64
1:E:35:ILE:H	1:E:35:ILE:HD13	1.63	0.64
1:E:118:ARG:HD3	1:E:146:GLN:O	1.97	0.64
1:B:37:LYS:HD2	3:B:1217:HOH:O	1.98	0.64
1:D:43:LYS:HB2	2:D:1203:RDL:O14	1.98	0.64
1:E:42:ILE:HG23	1:E:80:ALA:CB	2.28	0.63
1:A:146:GLN:NE2	1:A:146:GLN:HA	2.08	0.63
1:D:42:ILE:HG23	1:D:80:ALA:CB	2.29	0.63
1:B:42:ILE:HG23	1:B:80:ALA:CB	2.28	0.62
1:C:29:SER:HB2	3:C:1233:HOH:O	1.98	0.62
1:C:71:GLU:OE1	1:C:71:GLU:N	2.32	0.61
1:A:42:ILE:HG23	1:A:80:ALA:CB	2.28	0.61
1:A:7:ILE:HD12	1:A:22:ILE:HG12	1.82	0.60
1:E:4:LYS:HE2	1:E:35:ILE:HD12	1.82	0.60
1:D:25:LEU:C	1:D:32:ILE:HD11	2.21	0.60
1:C:14:ARG:HD2	1:E:152:GLY:O	2.01	0.60
1:B:7:ILE:HD12	1:B:22:ILE:HG12	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:GLY:HA3	3:D:1224:HOH:O	2.02	0.60
1:B:138:ARG:HG2	1:B:139:MET:HE2	1.83	0.60
1:B:14:ARG:NH2	3:B:1244:HOH:O	2.29	0.59
1:D:29:SER:OG	1:D:32:ILE:HG23	2.02	0.59
1:D:29:SER:HB3	1:D:32:ILE:HD13	1.85	0.59
1:A:68:GLY:HA3	1:A:73:ASP:OD2	2.03	0.58
1:C:21:ALA:CB	3:C:1248:HOH:O	2.51	0.57
1:A:22:ILE:HG23	1:A:34:ILE:HD13	1.84	0.57
1:C:50:LYS:NZ	1:E:92:ASN:HD21	2.01	0.57
1:E:2:THR:O	1:E:3:LYS:HB2	2.04	0.57
1:D:3:LYS:HD2	1:D:131:PHE:CE2	2.40	0.57
1:B:47:VAL:HG23	3:B:1221:HOH:O	2.03	0.57
1:E:22:ILE:CD1	1:E:36:ARG:HD2	2.35	0.57
1:D:14:ARG:HG3	1:D:66:MET:HE2	1.87	0.57
1:C:5:VAL:HB	1:C:34:ILE:CD1	2.36	0.56
1:A:14:ARG:HE	1:B:144:LEU:C	2.09	0.56
1:D:25:LEU:O	1:D:32:ILE:HD11	2.05	0.56
1:A:107:ASP:OD2	1:A:109:LYS:HB3	2.06	0.56
1:C:7:ILE:HD12	1:C:22:ILE:HG12	1.88	0.56
1:C:22:ILE:CD1	1:C:36:ARG:HD2	2.36	0.56
1:A:50:LYS:NZ	1:B:92:ASN:HD21	2.03	0.55
1:D:22:ILE:CD1	1:D:36:ARG:HD2	2.36	0.55
1:B:22:ILE:CD1	1:B:36:ARG:HD2	2.36	0.55
1:E:7:ILE:HD12	1:E:22:ILE:HG12	1.87	0.55
1:C:92:ASN:HD21	1:D:50:LYS:NZ	2.05	0.55
1:B:50:LYS:NZ	1:D:92:ASN:HD21	2.05	0.55
1:E:22:ILE:HG12	1:E:34:ILE:CD1	2.36	0.55
1:B:7:ILE:CD1	1:B:22:ILE:HG12	2.38	0.54
1:D:7:ILE:HD12	1:D:22:ILE:HG12	1.88	0.54
1:E:149:GLU:HG2	3:E:1245:HOH:O	2.06	0.54
1:C:118:ARG:HD3	1:C:146:GLN:O	2.07	0.54
1:A:42:ILE:HG22	1:A:43:LYS:N	2.23	0.54
1:E:42:ILE:HG22	1:E:43:LYS:N	2.23	0.54
1:B:42:ILE:HG22	1:B:43:LYS:N	2.23	0.54
1:B:143:GLY:O	1:B:144:LEU:CB	2.53	0.54
1:D:14:ARG:HB2	1:D:66:MET:CE	2.39	0.53
1:A:112:ASP:HB2	3:A:1244:HOH:O	2.07	0.53
1:C:71:GLU:CD	1:C:72:LYS:H	2.11	0.53
1:C:71:GLU:OE1	1:C:72:LYS:N	2.36	0.53
1:C:109:LYS:HG3	3:C:1231:HOH:O	2.08	0.53
1:C:42:ILE:HG22	1:C:43:LYS:N	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:ARG:HD2	2:E:1202:RDL:C4	2.38	0.53
1:B:13:ALA:O	1:D:141:GLY:HA2	2.08	0.53
1:B:14:ARG:HD2	3:D:1224:HOH:O	2.08	0.53
1:D:107:ASP:OD2	1:D:109:LYS:HB3	2.08	0.53
1:A:7:ILE:CD1	1:A:22:ILE:HG12	2.38	0.53
1:D:88:GLN:NE2	1:D:95:ILE:H	2.07	0.52
1:C:7:ILE:CD1	1:C:22:ILE:HG12	2.39	0.52
1:E:22:ILE:HD11	1:E:36:ARG:HD2	1.91	0.52
1:C:5:VAL:HB	1:C:34:ILE:HD12	1.91	0.52
1:C:138:ARG:HA	3:C:1218:HOH:O	2.09	0.52
1:D:14:ARG:CG	1:D:66:MET:HE2	2.39	0.52
1:D:22:ILE:HD11	1:D:36:ARG:HD2	1.91	0.52
1:A:100:VAL:HG21	1:A:115:ALA:HA	1.92	0.51
1:D:100:VAL:HG21	1:D:115:ALA:HA	1.92	0.51
1:B:12:PHE:HZ	2:B:1209:RDL:H14O	1.55	0.51
1:C:92:ASN:HD21	1:D:50:LYS:HZ3	1.59	0.51
1:A:92:ASN:HD21	1:E:50:LYS:NZ	2.08	0.51
1:E:100:VAL:HG21	1:E:115:ALA:HA	1.93	0.51
1:A:24:LYS:O	1:A:28:LEU:HG	2.11	0.51
1:E:35:ILE:N	1:E:35:ILE:HD13	2.24	0.51
1:D:42:ILE:HG22	1:D:43:LYS:N	2.24	0.51
1:C:100:VAL:HG21	1:C:115:ALA:HA	1.93	0.51
1:D:7:ILE:CD1	1:D:22:ILE:HG12	2.41	0.51
1:C:71:GLU:CG	1:C:72:LYS:N	2.75	0.50
1:B:22:ILE:HD11	1:B:36:ARG:HD2	1.93	0.50
1:C:143:GLY:HA2	1:D:12:PHE:O	2.12	0.50
1:E:7:ILE:CD1	1:E:22:ILE:HG12	2.42	0.50
1:C:50:LYS:HZ2	1:E:92:ASN:ND2	2.10	0.50
1:C:66:MET:HG3	1:C:100:VAL:O	2.12	0.49
1:E:88:GLN:NE2	1:E:95:ILE:H	2.09	0.49
1:E:34:ILE:HG12	1:E:35:ILE:N	2.27	0.49
1:C:26:LYS:HA	3:C:1241:HOH:O	2.12	0.49
1:B:72:LYS:O	1:B:75:VAL:N	2.44	0.49
2:A:1208:RDL:H14O	1:E:12:PHE:HZ	1.60	0.49
1:B:88:GLN:NE2	1:B:95:ILE:H	2.11	0.49
1:E:66:MET:HG3	1:E:100:VAL:O	2.12	0.48
1:B:100:VAL:HG21	1:B:115:ALA:HA	1.95	0.48
1:A:42:ILE:HA	1:A:42:ILE:HD13	1.68	0.48
1:B:50:LYS:HZ2	1:D:92:ASN:ND2	2.11	0.48
1:C:88:GLN:NE2	1:C:95:ILE:H	2.12	0.47
1:D:66:MET:HE3	1:D:102:GLU:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:ILE:HG13	1:D:116:LYS:HG2	1.96	0.47
1:C:22:ILE:HD11	1:C:36:ARG:HD2	1.96	0.47
1:C:71:GLU:HG2	1:C:72:LYS:N	2.30	0.47
1:B:28:LEU:HD13	1:B:127:TYR:CG	2.50	0.47
1:D:25:LEU:HB3	1:D:32:ILE:CD1	2.45	0.47
2:D:1203:RDL:C12	2:D:1203:RDL:HN1	2.27	0.46
1:C:12:PHE:O	1:E:143:GLY:HA2	2.14	0.46
1:A:68:GLY:H	1:A:73:ASP:HB3	1.80	0.46
1:A:92:ASN:HD21	1:E:50:LYS:HZ3	1.62	0.46
1:E:3:LYS:HA	1:E:59:ASP:OD1	2.15	0.46
1:D:69:LYS:HD3	1:D:102:GLU:HB2	1.97	0.46
1:C:86:LEU:CD1	1:E:86:LEU:HD21	2.46	0.46
1:A:32:ILE:HD13	1:A:34:ILE:HG13	1.97	0.45
1:B:42:ILE:HA	1:B:42:ILE:HD13	1.68	0.45
1:C:127:TYR:HE1	3:C:1233:HOH:O	1.98	0.45
1:C:45:LEU:HB2	1:C:46:PRO:HD3	1.97	0.45
1:B:107:ASP:HB2	3:B:1233:HOH:O	2.17	0.45
1:A:137:THR:HA	1:E:38:THR:OG1	2.17	0.45
1:E:118:ARG:CD	1:E:146:GLN:O	2.65	0.45
1:C:86:LEU:HD21	1:D:86:LEU:CD1	2.47	0.45
1:E:3:LYS:HD3	1:E:3:LYS:HA	1.79	0.45
1:A:116:LYS:NZ	3:A:1216:HOH:O	2.50	0.45
1:E:42:ILE:HB	2:E:1207:RDL:C2	2.47	0.44
1:D:68:GLY:HA3	1:D:73:ASP:OD1	2.17	0.44
1:A:88:GLN:NE2	1:A:95:ILE:H	2.16	0.44
1:A:38:THR:OG1	1:B:137:THR:HA	2.16	0.44
1:C:42:ILE:CG2	1:C:43:LYS:N	2.80	0.44
1:A:50:LYS:NZ	1:B:92:ASN:ND2	2.65	0.44
1:B:20:ILE:HG22	1:B:120:GLU:HB2	2.00	0.44
1:B:42:ILE:HB	2:B:1210:RDL:C2	2.47	0.44
1:C:50:LYS:NZ	1:E:92:ASN:ND2	2.66	0.44
1:C:71:GLU:O	1:C:74:LYS:HB2	2.17	0.44
1:E:20:ILE:HG13	1:E:116:LYS:HG2	1.99	0.44
1:E:29:SER:O	1:E:32:ILE:HG22	2.17	0.44
1:A:45:LEU:HB2	1:A:46:PRO:HD3	1.99	0.44
1:C:20:ILE:HG13	1:C:116:LYS:HG2	2.00	0.43
1:E:42:ILE:CG2	1:E:43:LYS:N	2.81	0.43
1:A:50:LYS:HZ2	1:B:92:ASN:ND2	2.15	0.43
1:A:117:ARG:NH2	1:A:120:GLU:OE2	2.47	0.43
1:B:42:ILE:CG2	1:B:43:LYS:N	2.81	0.43
1:A:42:ILE:CG2	1:A:43:LYS:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:47:VAL:CG2	1:E:88:GLN:CB	2.87	0.43
1:C:122:HIS:HE1	2:D:1203:RDL:O13	2.01	0.43
1:E:42:ILE:HA	1:E:42:ILE:HD13	1.70	0.43
1:D:42:ILE:HA	1:D:42:ILE:HD13	1.67	0.43
1:D:42:ILE:CG2	1:D:43:LYS:N	2.82	0.42
1:A:4:LYS:CE	1:A:35:ILE:HD12	2.49	0.42
1:B:50:LYS:NZ	1:D:92:ASN:ND2	2.66	0.42
1:B:71:GLU:HG2	3:B:1251:HOH:O	2.19	0.42
1:B:138:ARG:HG2	1:B:139:MET:CE	2.47	0.42
1:D:20:ILE:HG22	1:D:120:GLU:HB2	2.01	0.42
1:A:34:ILE:HG22	1:A:35:ILE:N	2.35	0.42
1:C:20:ILE:HG22	1:C:120:GLU:HB2	2.02	0.42
1:D:69:LYS:CD	1:D:102:GLU:HB2	2.50	0.42
1:A:92:ASN:ND2	1:E:50:LYS:NZ	2.68	0.42
1:E:69:LYS:O	1:E:70:ALA:C	2.58	0.42
1:C:33:LYS:O	1:C:34:ILE:HD13	2.19	0.42
1:A:29:SER:CB	1:A:32:ILE:HG23	2.49	0.42
1:C:42:ILE:HB	2:C:1201:RDL:C2	2.50	0.42
1:A:50:LYS:HZ3	1:B:92:ASN:HD21	1.67	0.42
1:D:25:LEU:HB3	1:D:32:ILE:HD12	2.02	0.41
1:E:20:ILE:HG22	1:E:120:GLU:HB2	2.02	0.41
1:A:34:ILE:CG2	1:A:35:ILE:N	2.83	0.41
1:C:29:SER:O	1:C:32:ILE:HG22	2.20	0.41
1:D:88:GLN:HE21	1:D:94:HIS:HA	1.85	0.41
1:E:70:ALA:O	1:E:73:ASP:HB2	2.21	0.41
1:E:69:LYS:O	1:E:70:ALA:O	2.38	0.41
1:D:69:LYS:HB2	3:D:1218:HOH:O	2.19	0.41
1:C:107:ASP:OD2	1:C:109:LYS:HB2	2.21	0.41
1:B:12:PHE:HZ	2:B:1209:RDL:O14	2.04	0.41
1:C:52:LEU:HA	1:C:52:LEU:HD12	1.90	0.41
1:D:117:ARG:HD2	1:D:117:ARG:HA	1.81	0.41
1:B:45:LEU:HB2	1:B:46:PRO:HD3	2.03	0.41
1:B:141:GLY:O	1:B:142:LYS:C	2.60	0.41
1:E:45:LEU:HB2	1:E:46:PRO:HD3	2.03	0.41
1:A:108:ASP:HA	1:A:111:LEU:HB3	2.02	0.41
1:C:88:GLN:HE21	1:C:94:HIS:HA	1.86	0.40
1:D:45:LEU:HB2	1:D:46:PRO:HD3	2.02	0.40
1:B:84:LEU:HD12	1:B:97:GLU:OE1	2.21	0.40
1:E:88:GLN:HE21	1:E:94:HIS:HA	1.86	0.40
1:A:47:VAL:CG2	1:B:88:GLN:CB	2.88	0.40
1:C:118:ARG:HD2	2:C:1204:RDL:C4	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ILE:HG23	1:A:34:ILE:HD12	2.00	0.40
1:C:122:HIS:CE1	2:D:1203:RDL:O13	2.75	0.40
1:B:4:LYS:HG3	1:B:33:LYS:HB2	2.04	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	144/156 (92%)	137 (95%)	6 (4%)	1 (1%)	26	25
1	B	141/156 (90%)	133 (94%)	7 (5%)	1 (1%)	26	25
1	C	150/156 (96%)	145 (97%)	4 (3%)	1 (1%)	26	25
1	D	139/156 (89%)	135 (97%)	3 (2%)	1 (1%)	26	25
1	E	150/156 (96%)	143 (95%)	6 (4%)	1 (1%)	26	25
All	All	724/780 (93%)	693 (96%)	26 (4%)	5 (1%)	26	25

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	70	ALA
1	C	70	ALA
1	B	142	LYS
1	A	145	ARG
1	D	70	ALA

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	123/130 (95%)	118 (96%)	5 (4%)	37	45
1	B	121/130 (93%)	117 (97%)	4 (3%)	45	55
1	C	127/130 (98%)	122 (96%)	5 (4%)	39	47
1	D	119/130 (92%)	116 (98%)	3 (2%)	55	67
1	E	127/130 (98%)	123 (97%)	4 (3%)	47	58
All	All	617/650 (95%)	596 (97%)	21 (3%)	44	54

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ILE
1	A	52	LEU
1	A	73	ASP
1	A	145	ARG
1	A	146	GLN
1	B	42	ILE
1	B	52	LEU
1	B	69	LYS
1	B	138	ARG
1	C	42	ILE
1	C	52	LEU
1	C	71	GLU
1	C	72	LYS
1	C	117	ARG
1	D	42	ILE
1	D	52	LEU
1	D	72	LYS
1	E	34	ILE
1	E	35	ILE
1	E	42	ILE
1	E	52	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	92	ASN

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Mol	Chain	Res	Type
1	A	146	GLN
1	B	88	GLN
1	B	92	ASN
1	C	88	GLN
1	C	92	ASN
1	D	88	GLN
1	D	92	ASN
1	E	88	GLN
1	E	92	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

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	RDL	A	1205	-	23,24,24	2.44	3 (13%)	19,35,35	1.49	3 (15%)
2	RDL	A	1208	-	23,24,24	2.41	3 (13%)	19,35,35	1.46	2 (10%)
2	RDL	B	1206	-	23,24,24	2.21	3 (13%)	19,35,35	1.38	2 (10%)
2	RDL	B	1209	-	23,24,24	2.44	3 (13%)	19,35,35	1.47	3 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	RDL	B	1210	-	23,24,24	2.52	4 (17%)	19,35,35	1.50	3 (15%)
2	RDL	C	1201	-	23,24,24	2.46	4 (17%)	19,35,35	1.50	2 (10%)
2	RDL	C	1204	-	23,24,24	2.43	4 (17%)	19,35,35	1.39	3 (15%)
2	RDL	D	1203	-	23,24,24	2.17	4 (17%)	19,35,35	1.59	2 (10%)
2	RDL	E	1202	-	23,24,24	2.44	4 (17%)	19,35,35	1.42	3 (15%)
2	RDL	E	1207	-	23,24,24	2.55	5 (21%)	19,35,35	1.48	3 (15%)

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	RDL	A	1205	-	-	0/14/46/46	0/2/2/2
2	RDL	A	1208	-	-	0/14/46/46	0/2/2/2
2	RDL	B	1206	-	-	0/14/46/46	0/2/2/2
2	RDL	B	1209	-	-	0/14/46/46	0/2/2/2
2	RDL	B	1210	-	-	0/14/46/46	0/2/2/2
2	RDL	C	1201	-	-	0/14/46/46	0/2/2/2
2	RDL	C	1204	-	-	0/14/46/46	0/2/2/2
2	RDL	D	1203	-	-	0/14/46/46	0/2/2/2
2	RDL	E	1202	-	-	0/14/46/46	0/2/2/2
2	RDL	E	1207	-	-	0/14/46/46	0/2/2/2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1210	RDL	C10-N9	-8.64	1.37	1.45
2	C	1201	RDL	C10-N9	-8.28	1.37	1.45
2	E	1207	RDL	C10-N9	-8.06	1.37	1.45
2	E	1202	RDL	C10-N9	-7.90	1.37	1.45
2	A	1205	RDL	C10-N9	-7.84	1.37	1.45
2	A	1208	RDL	C10-N9	-7.66	1.38	1.45
2	B	1209	RDL	C10-N9	-7.37	1.38	1.45
2	C	1204	RDL	C10-N9	-7.37	1.38	1.45
2	B	1209	RDL	C5-N6	-6.70	1.37	1.46
2	A	1208	RDL	C5-N6	-6.63	1.37	1.46
2	E	1207	RDL	C5-N6	-6.61	1.37	1.46
2	C	1204	RDL	C5-N6	-6.59	1.37	1.46
2	B	1206	RDL	C10-N9	-6.54	1.39	1.45
2	A	1205	RDL	C5-N6	-6.40	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1201	RDL	C5-N6	-6.36	1.38	1.46
2	D	1203	RDL	C5-N6	-6.24	1.38	1.46
2	D	1203	RDL	C10-N9	-6.20	1.39	1.45
2	B	1206	RDL	C5-N6	-6.20	1.38	1.46
2	E	1202	RDL	C5-N6	-6.18	1.38	1.46
2	B	1210	RDL	C5-N6	-6.01	1.38	1.46
2	E	1202	RDL	C5-C4	-4.64	1.44	1.53
2	B	1209	RDL	C5-C4	-4.32	1.45	1.53
2	E	1207	RDL	C5-C4	-4.02	1.45	1.53
2	A	1208	RDL	C5-C4	-3.99	1.45	1.53
2	C	1204	RDL	C5-C4	-3.88	1.46	1.53
2	A	1205	RDL	C5-C4	-3.85	1.46	1.53
2	B	1210	RDL	C5-C4	-3.83	1.46	1.53
2	B	1206	RDL	C5-C4	-3.81	1.46	1.53
2	C	1201	RDL	C5-C4	-3.78	1.46	1.53
2	D	1203	RDL	C5-C4	-3.64	1.46	1.53
2	E	1207	RDL	C11-C12	-2.44	1.48	1.52
2	C	1201	RDL	C8-C7	-2.10	1.49	1.53
2	B	1210	RDL	C11-C12	-2.03	1.49	1.52
2	D	1203	RDL	O7-C7	2.00	1.27	1.23
2	E	1207	RDL	O4-C4	2.06	1.27	1.23
2	E	1202	RDL	O7-C7	2.16	1.27	1.23
2	C	1204	RDL	O7-C7	2.27	1.27	1.23

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1208	RDL	O12-C12-C11	-2.71	104.05	110.45
2	B	1209	RDL	O12-C12-C11	-2.60	104.31	110.45
2	B	1210	RDL	O12-C12-C11	-2.56	104.40	110.45
2	E	1202	RDL	O12-C12-C11	-2.47	104.62	110.45
2	A	1205	RDL	O12-C12-C11	-2.36	104.87	110.45
2	E	1207	RDL	O12-C12-C11	-2.12	105.45	110.45
2	C	1204	RDL	O12-C12-C11	-2.08	105.53	110.45
2	E	1202	RDL	C7-C8-N9	2.02	119.16	117.61
2	B	1209	RDL	C7-C8-N9	2.19	119.29	117.61
2	B	1206	RDL	C7-C8-N9	2.27	119.35	117.61
2	A	1205	RDL	C7-C8-N9	2.30	119.37	117.61
2	C	1204	RDL	C7-C8-N9	2.31	119.38	117.61
2	E	1207	RDL	C7-C8-N9	2.33	119.40	117.61
2	C	1201	RDL	C7-C8-N9	2.38	119.44	117.61
2	B	1210	RDL	C7-C8-N9	2.46	119.49	117.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1203	RDL	C7-C8-N9	3.71	120.46	117.61
2	E	1202	RDL	N3-C2-N1	4.40	120.95	116.14
2	B	1206	RDL	N3-C2-N1	4.43	121.00	116.14
2	B	1210	RDL	N3-C2-N1	4.47	121.03	116.14
2	C	1204	RDL	N3-C2-N1	4.50	121.07	116.14
2	B	1209	RDL	N3-C2-N1	4.55	121.12	116.14
2	D	1203	RDL	N3-C2-N1	4.57	121.14	116.14
2	A	1208	RDL	N3-C2-N1	4.63	121.21	116.14
2	A	1205	RDL	N3-C2-N1	4.67	121.26	116.14
2	E	1207	RDL	N3-C2-N1	4.77	121.36	116.14
2	C	1201	RDL	N3-C2-N1	4.83	121.43	116.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1208	RDL	1	0
2	B	1209	RDL	2	0
2	B	1210	RDL	1	0
2	C	1201	RDL	1	0
2	C	1204	RDL	1	0
2	D	1203	RDL	6	0
2	E	1202	RDL	1	0
2	E	1207	RDL	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	146/156 (93%)	0.43	6 (4%)	41	39	19, 29, 41, 46	15 (10%)
1	B	143/156 (91%)	0.30	6 (4%)	40	39	20, 30, 41, 51	19 (13%)
1	C	152/156 (97%)	0.31	1 (0%)	89	88	18, 28, 38, 44	14 (9%)
1	D	141/156 (90%)	0.31	4 (2%)	56	56	17, 29, 39, 45	14 (9%)
1	E	152/156 (97%)	0.20	2 (1%)	79	78	18, 29, 39, 48	15 (9%)
All	All	734/780 (94%)	0.31	19 (2%)	59	59	17, 29, 40, 51	77 (10%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	16	ASP	4.1
1	B	143	GLY	3.6
1	D	143	GLY	3.5
1	A	30	PRO	3.3
1	A	70	ALA	3.2
1	E	152	GLY	2.8
1	B	138	ARG	2.6
1	A	103	ASP	2.6
1	D	20	ILE	2.5
1	A	2	THR	2.5
1	B	144	LEU	2.5
1	B	15	VAL	2.5
1	D	113	TRP	2.4
1	B	128	TYR	2.2
1	D	32	ILE	2.2
1	C	128	TYR	2.1
1	A	66	MET	2.1
1	E	133	PRO	2.1
1	B	135	TYR	2.0

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

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

6.3 Carbohydrates (i)

There are no 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	RDL	B	1209	23/23	0.66	0.31	5.75	59,64,70,70	0
2	RDL	C	1204	23/23	0.68	0.27	4.48	35,41,48,53	0
2	RDL	D	1203	23/23	0.78	0.24	2.75	32,40,58,61	0
2	RDL	A	1208	23/23	0.76	0.28	2.08	43,46,59,59	0
2	RDL	E	1207	23/23	0.84	0.17	1.19	24,31,33,37	0
2	RDL	B	1210	23/23	0.88	0.16	0.94	29,35,38,40	0
2	RDL	A	1205	23/23	0.85	0.18	0.33	26,35,38,39	0
2	RDL	E	1202	23/23	0.87	0.18	0.13	24,31,46,47	0
2	RDL	C	1201	23/23	0.90	0.15	-0.06	21,25,28,30	0
2	RDL	B	1206	23/23	-	-	-	15,15,15,15	23

6.5 Other polymers (i)

There are no such residues in this entry.