Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 05:54 AM GMT

PDB ID	:	2V4E
Title	:	A NON-CYTOTOXIC DSRED VARIANT FOR WHOLE-CELL LABELING
Authors	:	Strack, R.L.; Strongin, D.E.; Bhattacharyya, D.; Tao, W.; Berman, A.; Broxmeyer, H.E.; Keenan, R.J.; Glick, B.S.
Deposited on	:	2008-09-20
Resolution	:	2.40 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:

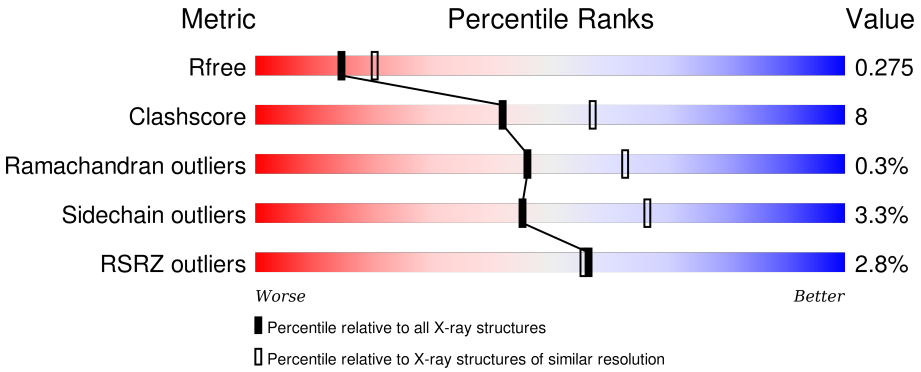
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	218	2% 85% 14%
2	B	218	% 80% 19%
3	C	218	2% 78% 19%
3	D	218	% 85% 11%
3	E	218	2% 83% 15%

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Mol	Chain	Length	Quality of chain
3	F	218	2% 85% 13%
3	G	218	11% 71% 27%
3	H	218	2% 87% 11%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14705 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 RED FLUORESCENT PROTEIN DRFP583.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1770	1150	290	323	7			

- Molecule 2 is a protein called RED FLUORESCENT PROTEIN DRFP583.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1779	1154	293	325	7			

- Molecule 3 is a protein called RED FLUORESCENT PROTEIN DRFP583.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	218	Total	C	N	O	S	0	0	0
			1779	1153	293	326	7			
3	D	218	Total	C	N	O	S	0	0	0
			1779	1153	293	326	7			
3	E	217	Total	C	N	O	S	0	0	0
			1770	1149	290	324	7			
3	F	218	Total	C	N	O	S	0	0	0
			1779	1153	293	326	7			
3	G	218	Total	C	N	O	S	0	0	0
			1779	1153	293	326	7			
3	H	218	Total	C	N	O	S	0	0	0
			1779	1153	293	326	7			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	63	Total	O	0	0
			63	63		
4	B	78	Total	O	0	0
			78	78		

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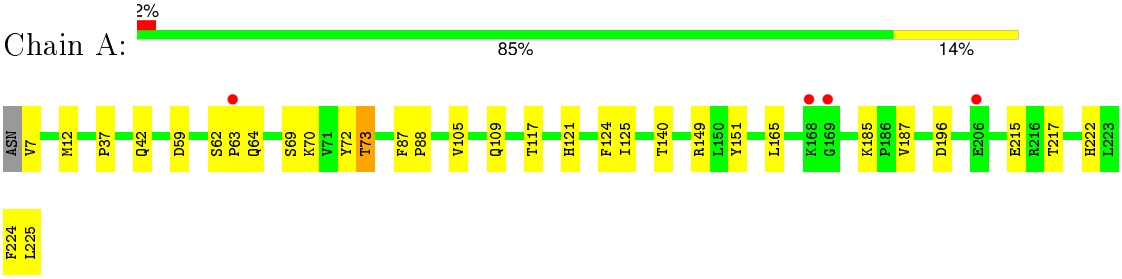
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	70	Total O 70 70	0	0
4	D	80	Total O 80 80	0	0
4	E	56	Total O 56 56	0	0
4	F	73	Total O 73 73	0	0
4	G	23	Total O 23 23	0	0
4	H	48	Total O 48 48	0	0

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.

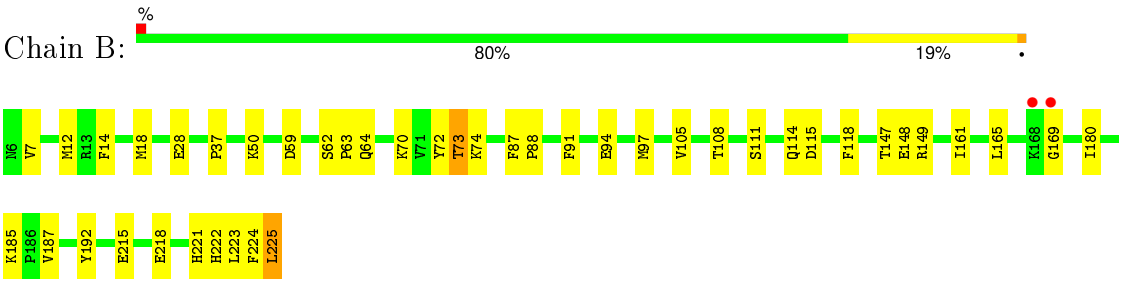
- Molecule 1: RED FLUORESCENT PROTEIN DRFP583

Chain A:



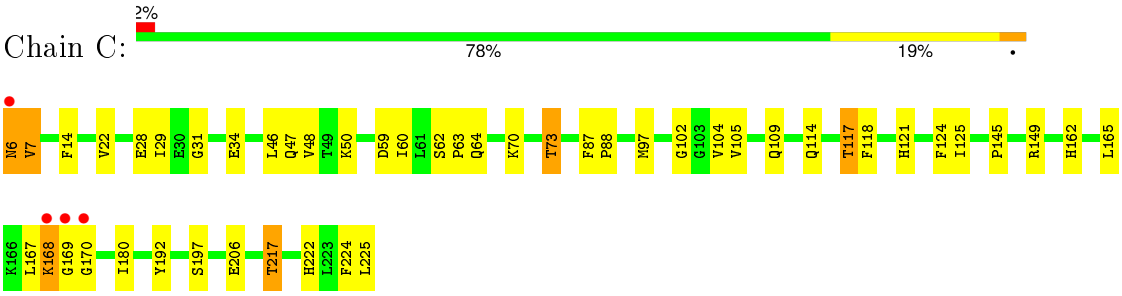
- Molecule 2: RED FLUORESCENT PROTEIN DRFP583

Chain B:



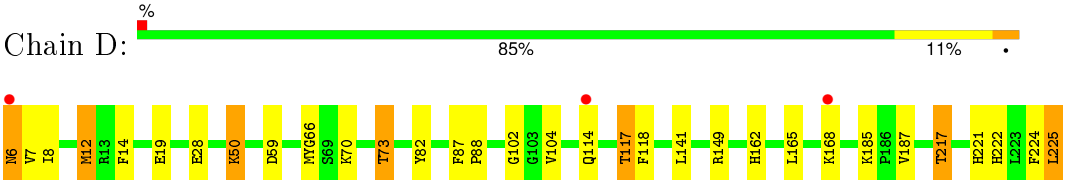
- Molecule 3: RED FLUORESCENT PROTEIN DRFP583

Chain C:



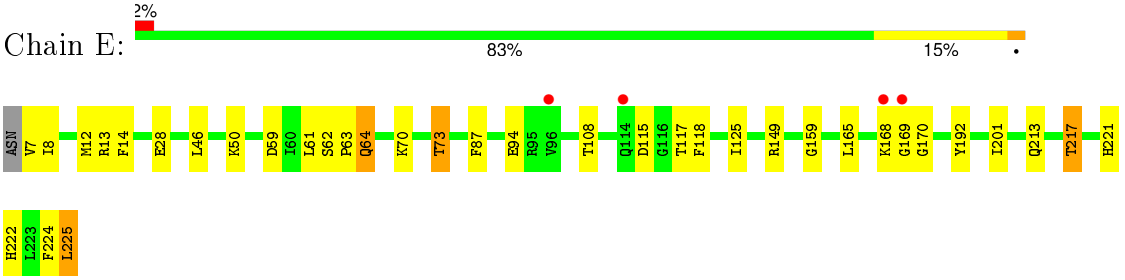
- Molecule 3: RED FLUORESCENT PROTEIN DRFP583

Chain D:



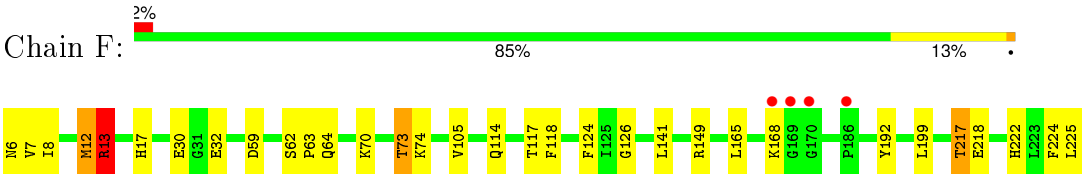
- Molecule 3: RED FLUORESCENT PROTEIN DRFP583

Chain E:



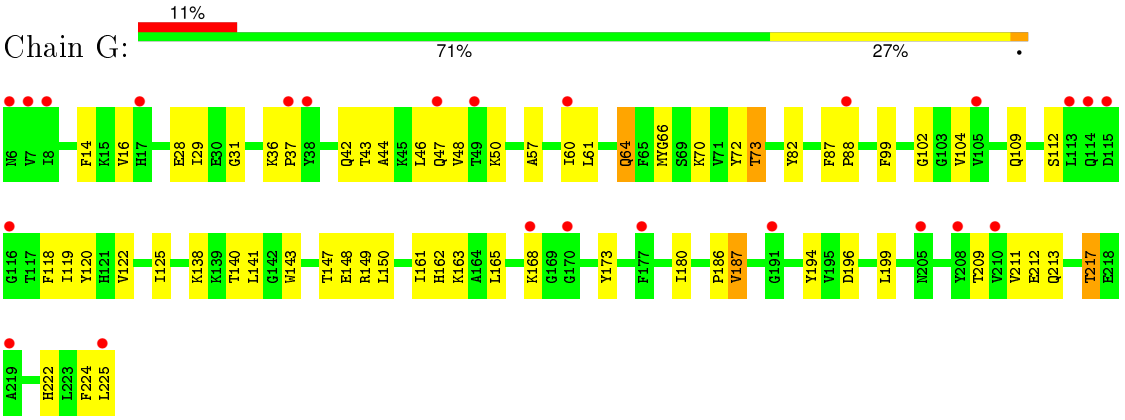
• Molecule 3: RED FLUORESCENT PROTEIN DRFP583

Chain F:



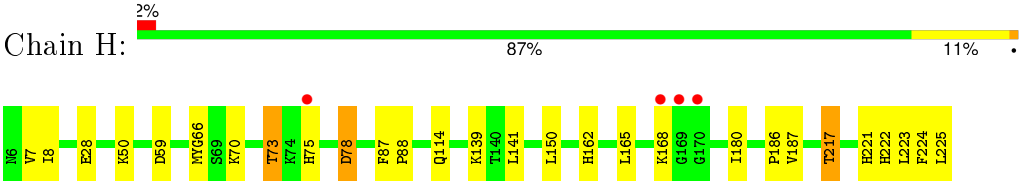
• Molecule 3: RED FLUORESCENT PROTEIN DRFP583

Chain G:



• Molecule 3: RED FLUORESCENT PROTEIN DRFP583

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	115.53Å 122.62Å 164.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 34.89 – 2.39	Depositor EDS
% Data completeness (in resolution range)	98.6 (50.00-2.40) 98.1 (34.89-2.39)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.65 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0053	Depositor
R, R_{free}	0.220 , 0.271 0.223 , 0.275	Depositor DCC
R_{free} test set	4523 reflections (5.24%)	DCC
Wilson B-factor (Å^2)	27.7	Xtriage
Anisotropy	0.686	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 91099 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14705	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: NRQ

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	0.57	0/1799	0.68	0/2425
2	B	0.62	0/1808	0.71	2/2439 (0.1%)
3	C	0.59	0/1808	0.67	0/2439
3	D	0.62	0/1808	0.70	1/2439 (0.0%)
3	E	0.52	0/1799	0.68	1/2426 (0.0%)
3	F	0.59	0/1808	0.72	4/2439 (0.2%)
3	G	0.57	0/1808	0.64	0/2439
3	H	0.57	0/1808	0.68	0/2439
All	All	0.58	0/14446	0.69	8/19485 (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	A	0	1
3	C	0	1
3	D	0	1
3	G	0	1
All	All	0	4

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	64	GLN	C-N-CA	-7.17	103.78	121.70
3	F	13	ARG	NE-CZ-NH1	7.01	123.80	120.30
3	D	225	LEU	CA-CB-CG	6.09	129.30	115.30
2	B	169	GLY	N-CA-C	-6.02	98.05	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	64	GLN	O-C-N	5.93	132.19	122.70
3	E	64	GLN	O-C-N	5.52	131.53	122.70
2	B	225	LEU	CA-CB-CG	5.36	127.62	115.30
3	F	64	GLN	CA-C-N	-5.00	106.19	117.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	64	GLN	Mainchain
3	C	64	GLN	Mainchain
3	D	6	ASN	Peptide
3	G	64	GLN	Mainchain

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	1770	0	1727	20	0
2	B	1779	0	1731	34	0
3	C	1779	0	1729	39	0
3	D	1779	0	1729	29	0
3	E	1770	0	1722	29	0
3	F	1779	0	1729	25	0
3	G	1779	0	1729	45	0
3	H	1779	0	1729	24	0
4	A	63	0	0	2	0
4	B	78	0	0	1	0
4	C	70	0	0	2	0
4	D	80	0	0	3	0
4	E	56	0	0	3	0
4	F	73	0	0	4	0
4	G	23	0	0	0	0
4	H	48	0	0	4	0
All	All	14705	0	13825	236	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 8.

All (236) 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)
3:C:6:ASN:O	3:C:7:VAL:CG2	1.94	1.15
3:H:217:THR:HG21	4:H:2045:HOH:O	1.55	1.03
3:C:6:ASN:O	3:C:7:VAL:HG22	1.53	1.02
3:C:6:ASN:C	3:C:7:VAL:HG23	1.88	0.92
3:C:6:ASN:O	3:C:7:VAL:HG23	1.68	0.90
3:F:13:ARG:HH11	3:F:13:ARG:HG2	1.37	0.88
3:H:222:HIS:H	3:H:225:LEU:HD12	1.38	0.88
3:C:70:LYS:O	3:C:73:THR:HG22	1.75	0.85
3:E:70:LYS:O	3:E:73:THR:CG2	2.25	0.84
3:H:168:LYS:NZ	4:H:2038:HOH:O	2.09	0.83
3:D:117:THR:HG23	4:D:2037:HOH:O	1.80	0.80
1:A:70:LYS:O	1:A:73:THR:HG22	1.80	0.79
3:D:70:LYS:O	3:D:73:THR:HG23	1.84	0.78
3:C:6:ASN:C	3:C:7:VAL:CG2	2.43	0.77
3:F:73:THR:HG21	4:F:2023:HOH:O	1.85	0.76
3:D:12:MET:HE2	3:D:118:PHE:CZ	2.21	0.76
2:B:70:LYS:O	2:B:73:THR:CG2	2.33	0.76
3:C:70:LYS:O	3:C:73:THR:CG2	2.34	0.74
3:H:70:LYS:O	3:H:73:THR:HG22	1.86	0.74
3:F:70:LYS:O	3:F:73:THR:CG2	2.36	0.73
3:H:70:LYS:O	3:H:73:THR:CG2	2.37	0.73
3:E:217:THR:HG21	4:E:2052:HOH:O	1.86	0.72
1:A:73:THR:HG21	4:A:2019:HOH:O	1.88	0.72
3:F:222:HIS:HD2	3:F:224:PHE:H	1.39	0.70
2:B:222:HIS:H	2:B:225:LEU:HD12	1.56	0.69
3:D:12:MET:CE	3:D:118:PHE:CZ	2.77	0.68
3:G:70:LYS:O	3:G:73:THR:HG23	1.92	0.68
3:F:70:LYS:O	3:F:73:THR:HG23	1.93	0.67
3:E:70:LYS:O	3:E:73:THR:HG23	1.94	0.67
3:F:141:LEU:HD11	3:F:168:LYS:HA	1.77	0.66
2:B:70:LYS:O	2:B:73:THR:HG23	1.95	0.65
3:F:17:HIS:HB2	4:F:2007:HOH:O	1.96	0.65
1:A:70:LYS:O	1:A:73:THR:CG2	2.45	0.65
3:C:168:LYS:O	3:C:170:GLY:N	2.30	0.64
3:H:222:HIS:N	3:H:225:LEU:HD12	2.10	0.63
3:D:6:ASN:N	3:D:7:VAL:CA	2.62	0.63
3:C:28:GLU:HB2	3:C:50:LYS:HB2	1.81	0.62
3:H:78:ASP:N	3:H:78:ASP:OD1	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:12:MET:HE3	3:E:118:PHE:CZ	2.35	0.61
3:E:7:VAL:CA	4:E:2001:HOH:O	2.47	0.61
3:E:70:LYS:O	3:E:73:THR:HG22	2.00	0.60
2:B:59:ASP:HB3	2:B:165:LEU:HD21	1.83	0.60
3:E:8:ILE:HA	3:E:12:MET:HE1	1.83	0.60
2:B:74:LYS:HB3	2:B:218:GLU:HG2	1.84	0.60
3:G:109:GLN:HG3	3:G:122:VAL:HG22	1.84	0.60
3:D:6:ASN:N	3:D:7:VAL:C	2.56	0.59
3:D:222:HIS:CD2	3:D:224:PHE:H	2.19	0.59
2:B:222:HIS:N	2:B:225:LEU:HD12	2.17	0.59
3:G:162:HIS:CE1	3:H:162:HIS:CE1	2.91	0.59
2:B:221:HIS:HB3	2:B:225:LEU:HD12	1.84	0.59
3:G:29:ILE:HG12	3:G:48:VAL:HG22	1.86	0.58
3:E:62:SER:OG	3:E:63:PRO:HD3	2.04	0.58
3:F:105:VAL:HG11	3:F:124:PHE:CE2	2.38	0.57
3:D:59:ASP:HB3	3:D:165:LEU:HD21	1.86	0.57
3:C:73:THR:HG23	4:C:2019:HOH:O	2.04	0.57
3:E:222:HIS:H	3:E:225:LEU:HD22	1.70	0.56
3:C:62:SER:OG	3:C:63:PRO:HD3	2.05	0.56
3:G:109:GLN:CG	3:G:122:VAL:HG22	2.35	0.56
3:C:168:LYS:C	3:C:170:GLY:H	2.08	0.56
3:G:141:LEU:HD11	3:G:168:LYS:HA	1.88	0.56
1:A:87:PHE:HB3	1:A:88:PRO:HA	1.88	0.55
2:B:225:LEU:CD1	4:B:2064:HOH:O	2.54	0.55
3:D:222:HIS:H	3:D:225:LEU:HD12	1.71	0.55
3:D:66:NRQ:HA31	3:D:66:NRQ:N1	2.22	0.55
3:G:180:ILE:N	3:G:180:ILE:HD12	2.21	0.55
3:C:31:GLY:HA3	3:C:46:LEU:HD13	1.89	0.54
3:E:61:LEU:O	3:E:64:GLN:HG2	2.08	0.54
3:D:217:THR:CG2	4:D:2012:HOH:O	2.57	0.53
3:C:167:LEU:O	3:C:168:LYS:C	2.44	0.53
3:G:29:ILE:CG1	3:G:48:VAL:HG22	2.39	0.53
1:A:222:HIS:H	1:A:225:LEU:HD12	1.74	0.53
2:B:12:MET:CE	2:B:118:PHE:CZ	2.92	0.53
1:A:185:LYS:O	1:A:187:VAL:HG13	2.09	0.52
3:G:57:ALA:HB2	3:G:138:LYS:HA	1.90	0.52
3:E:222:HIS:CD2	3:E:224:PHE:H	2.27	0.52
3:G:16:VAL:HG23	3:G:120:TYR:CB	2.39	0.52
3:G:16:VAL:HG23	3:G:120:TYR:HB2	1.92	0.52
3:C:197:SER:OG	3:C:217:THR:HG23	2.10	0.52
3:D:222:HIS:N	3:D:225:LEU:HD12	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:222:HIS:H	3:C:225:LEU:HD12	1.76	0.51
3:H:139:LYS:HD2	3:H:168:LYS:HD2	1.92	0.51
2:B:180:ILE:HD12	2:B:180:ILE:N	2.25	0.51
3:F:8:ILE:HD12	3:F:8:ILE:N	2.25	0.51
3:F:141:LEU:CD1	3:F:168:LYS:HA	2.41	0.51
2:B:147:THR:O	2:B:161:ILE:HG23	2.09	0.51
2:B:221:HIS:HB3	2:B:225:LEU:CD1	2.41	0.50
1:A:222:HIS:CD2	1:A:224:PHE:H	2.29	0.50
1:A:37:PRO:HA	1:A:72:TYR:HA	1.93	0.50
3:D:82:TYR:CD1	3:D:187:VAL:CG2	2.94	0.50
3:C:162:HIS:CE1	3:D:162:HIS:CE1	2.99	0.50
3:G:82:TYR:CD1	3:G:187:VAL:CG2	2.94	0.50
3:E:222:HIS:HD2	3:E:224:PHE:H	1.59	0.50
1:A:125:ILE:HD12	3:C:125:ILE:HD12	1.94	0.50
3:F:13:ARG:HG2	3:F:13:ARG:NH1	2.14	0.50
3:C:167:LEU:O	3:C:168:LYS:O	2.30	0.49
3:D:102:GLY:O	3:D:104:VAL:HG23	2.12	0.49
1:A:105:VAL:HG11	1:A:124:PHE:CE2	2.47	0.49
3:G:14:PHE:CB	3:G:118:PHE:HB2	2.42	0.49
1:A:59:ASP:HB3	1:A:165:LEU:HD21	1.93	0.49
3:G:147:THR:O	3:G:161:ILE:HG23	2.12	0.49
3:F:74:LYS:HB3	3:F:218:GLU:HG2	1.94	0.49
3:H:87:PHE:HB3	3:H:88:PRO:HA	1.94	0.49
2:B:28:GLU:HB2	2:B:50:LYS:HB2	1.95	0.49
3:F:12:MET:HE2	3:F:118:PHE:CE2	2.47	0.49
2:B:12:MET:HE3	2:B:118:PHE:CZ	2.48	0.49
3:C:14:PHE:HB3	3:C:118:PHE:HB2	1.95	0.49
3:E:12:MET:CE	3:E:118:PHE:CZ	2.95	0.49
3:H:225:LEU:HD13	4:H:2046:HOH:O	2.11	0.49
3:F:222:HIS:CD2	3:F:224:PHE:H	2.27	0.49
3:F:222:HIS:HB3	3:F:225:LEU:HG	1.94	0.49
3:D:6:ASN:N	3:D:7:VAL:HA	2.28	0.48
3:D:149:ARG:C	3:D:149:ARG:HD2	2.33	0.48
3:D:6:ASN:N	3:D:8:ILE:N	2.61	0.48
3:C:222:HIS:CD2	3:C:224:PHE:H	2.31	0.48
3:G:87:PHE:HB3	3:G:88:PRO:HA	1.96	0.48
2:B:37:PRO:HA	2:B:72:TYR:HA	1.96	0.48
3:G:72:TYR:O	3:G:217:THR:HG23	2.13	0.48
3:G:222:HIS:CD2	3:G:224:PHE:H	2.31	0.48
3:E:125:ILE:HD12	3:G:125:ILE:HD12	1.96	0.48
2:B:222:HIS:CD2	2:B:224:PHE:H	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:28:GLU:HB2	3:H:50:LYS:HB2	1.95	0.47
3:G:222:HIS:H	3:G:225:LEU:HD12	1.80	0.47
2:B:148:GLU:HG3	2:B:161:ILE:HG12	1.97	0.47
3:G:140:THR:HG21	3:G:165:LEU:HD13	1.96	0.47
3:F:217:THR:CG2	4:F:2068:HOH:O	2.63	0.47
3:H:73:THR:HB	3:H:217:THR:OG1	2.15	0.46
3:E:8:ILE:HD11	3:E:87:PHE:HB2	1.97	0.46
3:G:147:THR:HG22	3:G:194:TYR:HD2	1.79	0.46
3:E:149:ARG:HD3	3:E:192:TYR:CZ	2.51	0.46
3:E:221:HIS:HB3	3:E:225:LEU:HD23	1.98	0.46
3:D:12:MET:HE3	3:D:118:PHE:CZ	2.49	0.46
3:H:8:ILE:HD11	3:H:87:PHE:HB2	1.96	0.46
3:G:61:LEU:O	3:G:64:GLN:HG2	2.15	0.46
3:G:82:TYR:CD1	3:G:187:VAL:HG22	2.51	0.46
3:E:168:LYS:C	3:E:170:GLY:H	2.18	0.46
3:E:94:GLU:HG2	3:E:108:THR:HA	1.98	0.46
3:E:14:PHE:HB3	3:E:118:PHE:HB2	1.98	0.46
2:B:14:PHE:CB	2:B:118:PHE:HB2	2.45	0.46
3:D:82:TYR:CD1	3:D:187:VAL:HG23	2.50	0.46
2:B:12:MET:HE2	2:B:118:PHE:CZ	2.51	0.46
3:C:145:PRO:HB2	3:D:222:HIS:CD2	2.51	0.45
3:E:46:LEU:N	3:E:46:LEU:HD22	2.31	0.45
3:H:186:PRO:O	3:H:187:VAL:HG12	2.16	0.45
3:C:149:ARG:HD3	3:C:192:TYR:CZ	2.52	0.45
2:B:70:LYS:NZ	2:B:215:GLU:OE2	2.43	0.45
2:B:149:ARG:HD3	2:B:192:TYR:CZ	2.51	0.45
3:G:149:ARG:C	3:G:149:ARG:HD2	2.36	0.45
2:B:18:MET:CE	2:B:64:GLN:HB2	2.46	0.45
3:F:105:VAL:HG11	3:F:124:PHE:CZ	2.51	0.45
2:B:94:GLU:HG2	2:B:108:THR:HA	1.98	0.45
3:D:73:THR:HG21	4:D:2029:HOH:O	2.17	0.45
1:A:140:THR:HG21	1:A:165:LEU:HD13	1.99	0.45
3:G:66:NRQ:HA31	3:G:66:NRQ:N1	2.32	0.45
3:F:70:LYS:O	3:F:73:THR:HG22	2.14	0.45
3:G:102:GLY:O	3:G:104:VAL:HG23	2.17	0.45
3:H:180:ILE:HD12	3:H:180:ILE:N	2.31	0.45
2:B:185:LYS:O	2:B:187:VAL:HG13	2.16	0.45
3:H:222:HIS:CD2	3:H:224:PHE:H	2.35	0.45
3:H:141:LEU:HD11	3:H:168:LYS:HA	1.98	0.45
3:F:217:THR:HG22	4:F:2068:HOH:O	2.17	0.45
3:C:114:GLN:O	3:C:117:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:MET:HE3	2:B:118:PHE:CE2	2.52	0.45
3:G:42:GLN:HG3	3:G:66:NRQ:CE	2.47	0.44
3:G:28:GLU:HB2	3:G:50:LYS:HB3	1.98	0.44
3:H:78:ASP:OD2	3:H:221:HIS:NE2	2.42	0.44
3:D:221:HIS:HB3	3:D:225:LEU:HD12	1.99	0.44
2:B:149:ARG:HD2	2:B:149:ARG:C	2.37	0.44
3:F:59:ASP:HB3	3:F:165:LEU:HD21	1.98	0.44
1:A:196:ASP:OD2	2:B:223:LEU:HD12	2.17	0.44
3:G:143:TRP:CE3	3:G:163:LYS:HE3	2.52	0.44
3:E:168:LYS:O	3:E:170:GLY:N	2.51	0.44
3:G:43:THR:HA	3:G:213:GLN:O	2.18	0.44
1:A:215:GLU:OE2	1:A:217:THR:OG1	2.34	0.44
1:A:109:GLN:HA	1:A:121:HIS:O	2.18	0.44
1:A:62:SER:N	1:A:63:PRO:CD	2.81	0.44
1:A:42:GLN:HE22	1:A:69:SER:HB3	1.82	0.44
3:C:180:ILE:HD12	3:C:180:ILE:N	2.33	0.44
2:B:91:PHE:O	2:B:111:SER:HB2	2.18	0.44
3:C:97:MET:HB2	3:C:105:VAL:HB	1.98	0.44
3:E:28:GLU:HB2	3:E:50:LYS:HB2	2.00	0.43
3:H:7:VAL:HG23	3:H:8:ILE:HD12	1.99	0.43
3:G:143:TRP:CE2	3:G:165:LEU:HD21	2.53	0.43
3:C:222:HIS:HD2	3:C:224:PHE:H	1.65	0.43
3:C:222:HIS:HB3	3:C:225:LEU:HG	2.00	0.43
3:G:196:ASP:OD2	3:H:223:LEU:HD12	2.18	0.43
3:H:66:NRQ:CB2	3:H:70:LYS:HE2	2.48	0.43
1:A:7:VAL:CA	4:A:2001:HOH:O	2.66	0.43
2:B:222:HIS:HD2	2:B:224:PHE:H	1.66	0.43
3:C:87:PHE:HB3	3:C:88:PRO:HA	2.01	0.43
3:C:14:PHE:CB	3:C:118:PHE:HB2	2.49	0.43
3:G:112:SER:O	3:G:119:ILE:N	2.45	0.43
3:D:141:LEU:HD11	3:D:168:LYS:HA	2.00	0.43
1:A:151:TYR:N	1:A:151:TYR:CD1	2.86	0.43
3:C:109:GLN:HA	3:C:121:HIS:O	2.19	0.43
3:C:225:LEU:CD1	4:C:2057:HOH:O	2.67	0.42
3:C:168:LYS:C	3:C:170:GLY:N	2.72	0.42
3:G:82:TYR:CE1	3:G:187:VAL:HG22	2.55	0.42
3:C:29:ILE:HG12	3:C:48:VAL:HG22	2.00	0.42
1:A:149:ARG:HD2	1:A:149:ARG:C	2.40	0.42
3:G:31:GLY:HA3	3:G:46:LEU:HD13	2.00	0.42
3:E:217:THR:CG2	4:E:2051:HOH:O	2.67	0.42
3:C:102:GLY:O	3:C:104:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:MET:HB2	2:B:105:VAL:HB	2.01	0.42
3:E:149:ARG:O	3:E:159:GLY:HA2	2.20	0.42
3:G:42:GLN:HG3	3:G:66:NRQ:HE1A	2.02	0.42
3:G:99:PHE:CD2	3:G:173:TYR:CE2	3.08	0.42
3:E:201:ILE:HD13	3:E:213:GLN:HG2	2.00	0.42
2:B:70:LYS:O	2:B:73:THR:HG22	2.14	0.42
3:C:22:VAL:HG21	3:C:60:ILE:HD11	2.02	0.42
3:H:59:ASP:HB3	3:H:165:LEU:HD21	2.02	0.42
3:G:36:LYS:HA	3:G:37:PRO:HD3	1.93	0.42
2:B:62:SER:OG	2:B:63:PRO:HD3	2.20	0.42
3:E:125:ILE:CD1	3:G:125:ILE:HD12	2.49	0.42
3:D:14:PHE:HB3	3:D:118:PHE:HB2	2.02	0.41
3:F:199:LEU:C	3:F:199:LEU:HD23	2.40	0.41
3:G:44:ALA:O	3:G:212:GLU:HA	2.20	0.41
3:G:143:TRP:CD2	3:G:165:LEU:HD21	2.55	0.41
3:F:105:VAL:HG22	3:F:126:GLY:HA2	2.02	0.41
3:D:87:PHE:HB3	3:D:88:PRO:HA	2.02	0.41
3:F:62:SER:N	3:F:63:PRO:CD	2.84	0.41
2:B:14:PHE:HB3	2:B:118:PHE:HB2	2.03	0.41
3:F:12:MET:CE	3:F:118:PHE:CZ	3.04	0.41
3:E:125:ILE:HG13	3:G:125:ILE:HD12	2.03	0.41
3:D:28:GLU:HB2	3:D:50:LYS:HB2	2.02	0.41
3:H:225:LEU:CD1	4:H:2046:HOH:O	2.68	0.41
3:C:105:VAL:HG11	3:C:124:PHE:CE2	2.56	0.41
3:E:59:ASP:HB3	3:E:165:LEU:HD21	2.03	0.41
3:G:14:PHE:HB3	3:G:118:PHE:HB2	2.03	0.40
3:G:148:GLU:O	3:G:150:LEU:HD12	2.21	0.40
3:G:66:NRQ:HE2	3:G:199:LEU:HB2	2.03	0.40
3:D:222:HIS:HD2	3:D:224:PHE:H	1.67	0.40
3:C:59:ASP:HB3	3:C:165:LEU:HD21	2.03	0.40
3:C:62:SER:N	3:C:63:PRO:CD	2.85	0.40
3:D:19:GLU:HG2	3:D:28:GLU:HG2	2.03	0.40
3:F:149:ARG:HD3	3:F:192:TYR:CZ	2.57	0.40
2:B:87:PHE:HB3	2:B:88:PRO:HA	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	212/218 (97%)	207 (98%)	5 (2%)	0	100 100
2	B	213/218 (98%)	210 (99%)	3 (1%)	0	100 100
3	C	213/218 (98%)	206 (97%)	4 (2%)	3 (1%)	14 19
3	D	213/218 (98%)	210 (99%)	3 (1%)	0	100 100
3	E	212/218 (97%)	205 (97%)	6 (3%)	1 (0%)	34 48
3	F	213/218 (98%)	209 (98%)	4 (2%)	0	100 100
3	G	213/218 (98%)	206 (97%)	6 (3%)	1 (0%)	34 48
3	H	213/218 (98%)	205 (96%)	8 (4%)	0	100 100
All	All	1702/1744 (98%)	1658 (97%)	39 (2%)	5 (0%)	46 63

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	7	VAL
3	C	168	LYS
3	C	169	GLY
3	E	169	GLY
3	G	186	PRO

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	188/190 (99%)	185 (98%)	3 (2%)	70 86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	190/190 (100%)	186 (98%)	4 (2%)	61 80
3	C	190/190 (100%)	183 (96%)	7 (4%)	41 62
3	D	190/190 (100%)	183 (96%)	7 (4%)	41 62
3	E	188/190 (99%)	182 (97%)	6 (3%)	46 68
3	F	190/190 (100%)	180 (95%)	10 (5%)	28 44
3	G	190/190 (100%)	183 (96%)	7 (4%)	41 62
3	H	190/190 (100%)	184 (97%)	6 (3%)	46 68
All	All	1516/1520 (100%)	1466 (97%)	50 (3%)	45 66

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	MET
1	A	73	THR
1	A	117	THR
2	B	7	VAL
2	B	73	THR
2	B	114	GLN
2	B	115	ASP
3	C	6	ASN
3	C	34	GLU
3	C	47	GLN
3	C	73	THR
3	C	117	THR
3	C	206	GLU
3	C	217	THR
3	D	12	MET
3	D	50	LYS
3	D	73	THR
3	D	114	GLN
3	D	117	THR
3	D	185	LYS
3	D	217	THR
3	E	13	ARG
3	E	73	THR
3	E	115	ASP
3	E	117	THR
3	E	217	THR
3	E	225	LEU
3	F	6	ASN

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Mol	Chain	Res	Type
3	F	7	VAL
3	F	12	MET
3	F	13	ARG
3	F	30	GLU
3	F	32	GLU
3	F	73	THR
3	F	114	GLN
3	F	117	THR
3	F	217	THR
3	G	47	GLN
3	G	60	ILE
3	G	73	THR
3	G	187	VAL
3	G	209	THR
3	G	211	VAL
3	G	217	THR
3	H	73	THR
3	H	75	HIS
3	H	78	ASP
3	H	114	GLN
3	H	150	LEU
3	H	217	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	HIS
2	B	47	GLN
2	B	222	HIS
3	C	6	ASN
3	C	222	HIS
3	D	222	HIS
3	E	121	HIS
3	E	222	HIS
3	F	222	HIS
3	G	121	HIS
3	G	222	HIS
3	H	47	GLN
3	H	162	HIS
3	H	222	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	NRQ	A	66	1	23,24,25	2.59	7 (30%)	23,32,34	3.09	7 (30%)
2	NRQ	B	66	2	23,24,25	2.70	6 (26%)	23,32,34	3.39	7 (30%)
3	NRQ	C	66	3	23,24,25	2.74	7 (30%)	23,32,34	2.96	7 (30%)
3	NRQ	D	66	3	23,24,25	2.66	6 (26%)	23,32,34	3.54	9 (39%)
3	NRQ	E	66	3	23,24,25	2.78	7 (30%)	23,32,34	3.52	7 (30%)
3	NRQ	F	66	3	23,24,25	2.62	7 (30%)	23,32,34	2.86	7 (30%)
3	NRQ	G	66	3	23,24,25	2.61	5 (21%)	23,32,34	3.31	7 (30%)
3	NRQ	H	66	3	23,24,25	2.84	7 (30%)	23,32,34	3.47	8 (34%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	NRQ	A	66	1	-	0/9/31/32	0/2/2/2
2	NRQ	B	66	2	-	0/9/31/32	0/2/2/2
3	NRQ	C	66	3	-	0/9/31/32	0/2/2/2
3	NRQ	D	66	3	-	0/9/31/32	0/2/2/2
3	NRQ	E	66	3	-	0/9/31/32	0/2/2/2
3	NRQ	F	66	3	-	0/9/31/32	0/2/2/2
3	NRQ	G	66	3	-	0/9/31/32	0/2/2/2
3	NRQ	H	66	3	-	0/9/31/32	0/2/2/2

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	66	NRQ	CA2-C2	-8.62	1.39	1.48
3	F	66	NRQ	CA2-C2	-8.17	1.39	1.48
3	H	66	NRQ	CA2-C2	-8.06	1.39	1.48
3	C	66	NRQ	CA2-C2	-7.91	1.40	1.48
2	B	66	NRQ	CA2-C2	-7.82	1.40	1.48
3	G	66	NRQ	CA2-C2	-7.29	1.40	1.48
3	D	66	NRQ	CA2-C2	-6.83	1.41	1.48
1	A	66	NRQ	CA2-C2	-6.76	1.41	1.48
2	B	66	NRQ	OH-CZ	-5.86	1.23	1.37
3	G	66	NRQ	OH-CZ	-5.79	1.23	1.37
3	C	66	NRQ	OH-CZ	-5.78	1.23	1.37
3	H	66	NRQ	OH-CZ	-5.74	1.23	1.37
3	E	66	NRQ	OH-CZ	-5.65	1.23	1.37
3	F	66	NRQ	OH-CZ	-5.47	1.24	1.37
1	A	66	NRQ	OH-CZ	-5.37	1.24	1.37
3	D	66	NRQ	OH-CZ	-4.94	1.25	1.37
3	H	66	NRQ	C2-N3	-3.80	1.31	1.39
3	F	66	NRQ	CG2-CB2	-3.21	1.40	1.46
3	C	66	NRQ	C2-N3	-3.14	1.33	1.39
3	E	66	NRQ	CG2-CB2	-3.09	1.40	1.46
1	A	66	NRQ	C2-N3	-3.08	1.33	1.39
3	E	66	NRQ	C2-N3	-3.06	1.33	1.39
3	F	66	NRQ	C2-N3	-2.97	1.33	1.39
3	C	66	NRQ	C1-N3	-2.85	1.33	1.38
3	D	66	NRQ	C1-N3	-2.77	1.33	1.38
3	D	66	NRQ	C2-N3	-2.71	1.34	1.39
3	H	66	NRQ	C1-N3	-2.68	1.33	1.38
3	E	66	NRQ	C1-N3	-2.63	1.33	1.38
3	G	66	NRQ	CG2-CB2	-2.61	1.41	1.46
2	B	66	NRQ	CG2-CB2	-2.51	1.41	1.46
3	C	66	NRQ	CG2-CB2	-2.45	1.41	1.46
3	H	66	NRQ	CG2-CB2	-2.37	1.42	1.46
2	B	66	NRQ	C1-N3	-2.32	1.34	1.38
1	A	66	NRQ	C1-N3	-2.32	1.34	1.38
3	H	66	NRQ	CA2-N2	-2.28	1.33	1.38
3	F	66	NRQ	CA2-N2	-2.26	1.33	1.38
3	D	66	NRQ	CG2-CB2	-2.24	1.42	1.46
3	G	66	NRQ	C2-N3	-2.23	1.35	1.39
3	C	66	NRQ	CA2-N2	-2.18	1.33	1.38
1	A	66	NRQ	CG2-CB2	-2.17	1.42	1.46
3	F	66	NRQ	C1-N3	-2.13	1.34	1.38
3	E	66	NRQ	CA2-N2	-2.12	1.33	1.38
2	B	66	NRQ	C2-N3	-2.06	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	NRQ	CA2-N2	-2.04	1.34	1.38
3	F	66	NRQ	CB2-CA2	5.32	1.39	1.35
3	E	66	NRQ	CB2-CA2	5.92	1.40	1.35
3	G	66	NRQ	CB2-CA2	6.23	1.40	1.35
3	C	66	NRQ	CB2-CA2	6.55	1.40	1.35
3	H	66	NRQ	CB2-CA2	6.82	1.41	1.35
1	A	66	NRQ	CB2-CA2	6.98	1.41	1.35
2	B	66	NRQ	CB2-CA2	7.07	1.41	1.35
3	D	66	NRQ	CB2-CA2	7.77	1.42	1.35

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	66	NRQ	O2-C2-CA2	-9.97	125.56	130.95
3	G	66	NRQ	O2-C2-CA2	-9.56	125.78	130.95
3	E	66	NRQ	O2-C2-CA2	-8.65	126.27	130.95
3	D	66	NRQ	O2-C2-CA2	-8.04	126.61	130.95
3	C	66	NRQ	O2-C2-CA2	-6.91	127.22	130.95
3	H	66	NRQ	O2-C2-CA2	-6.46	127.46	130.95
3	F	66	NRQ	O2-C2-CA2	-6.42	127.48	130.95
3	H	66	NRQ	C2-CA2-N2	-6.10	104.04	108.91
3	D	66	NRQ	C2-CA2-N2	-5.86	104.23	108.91
1	A	66	NRQ	C2-CA2-N2	-5.54	104.49	108.91
3	F	66	NRQ	N3-C1-N2	-5.39	107.16	113.26
2	B	66	NRQ	N3-C1-N2	-5.33	107.22	113.26
2	B	66	NRQ	C2-CA2-N2	-5.02	104.91	108.91
1	A	66	NRQ	N3-C1-N2	-4.97	107.63	113.26
3	H	66	NRQ	N3-C1-N2	-4.94	107.67	113.26
3	C	66	NRQ	C2-CA2-N2	-4.85	105.04	108.91
3	E	66	NRQ	C2-CA2-N2	-4.68	105.18	108.91
3	E	66	NRQ	N3-C1-N2	-4.63	108.02	113.26
1	A	66	NRQ	O2-C2-CA2	-4.60	128.46	130.95
3	C	66	NRQ	N3-C1-N2	-4.57	108.08	113.26
3	D	66	NRQ	N3-C1-N2	-4.56	108.09	113.26
3	G	66	NRQ	C2-CA2-N2	-4.21	105.55	108.91
3	F	66	NRQ	C2-CA2-N2	-4.15	105.60	108.91
3	G	66	NRQ	N3-C1-N2	-3.96	108.77	113.26
3	D	66	NRQ	CB1-CA1-N1	-3.14	119.16	124.94
2	B	66	NRQ	CB1-CA1-N1	-3.13	119.18	124.94
1	A	66	NRQ	CB1-CA1-N1	-3.11	119.22	124.94
3	E	66	NRQ	CB1-CA1-N1	-3.01	119.40	124.94
3	F	66	NRQ	CB1-CA1-N1	-2.98	119.47	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	66	NRQ	CB1-CA1-N1	-2.94	119.53	124.94
3	C	66	NRQ	CB1-CA1-N1	-2.94	119.54	124.94
3	G	66	NRQ	CB1-CA1-N1	-2.77	119.84	124.94
2	B	66	NRQ	CB1-CG1-SD	-2.64	106.41	112.88
3	H	66	NRQ	CB1-CG1-SD	-2.07	107.81	112.88
3	D	66	NRQ	CE1-CZ-CE2	-2.02	116.91	119.79
1	A	66	NRQ	CB2-CA2-N2	2.10	132.43	128.67
3	F	66	NRQ	C3-CA3-N3	2.33	118.11	113.00
3	H	66	NRQ	C3-CA3-N3	2.35	118.15	113.00
3	D	66	NRQ	CD1-CE1-CZ	2.35	122.59	119.87
3	G	66	NRQ	CB2-CA2-N2	2.37	132.90	128.67
3	C	66	NRQ	CB2-CA2-N2	2.51	133.16	128.67
3	D	66	NRQ	CB2-CA2-N2	2.51	133.16	128.67
3	F	66	NRQ	CB2-CA2-N2	2.55	133.23	128.67
3	G	66	NRQ	C3-CA3-N3	2.85	119.24	113.00
3	H	66	NRQ	CB2-CA2-N2	2.86	133.78	128.67
2	B	66	NRQ	CB2-CA2-N2	3.10	134.21	128.67
3	C	66	NRQ	C3-CA3-N3	3.11	119.82	113.00
3	D	66	NRQ	C3-CA3-N3	3.41	120.46	113.00
3	E	66	NRQ	CB2-CA2-N2	3.42	134.78	128.67
1	A	66	NRQ	C3-CA3-N3	4.10	121.98	113.00
3	E	66	NRQ	C3-CA3-N3	4.19	122.17	113.00
3	F	66	NRQ	CA2-C2-N3	8.00	107.41	103.40
3	C	66	NRQ	CA2-C2-N3	8.68	107.75	103.40
2	B	66	NRQ	CA2-C2-N3	8.90	107.86	103.40
3	G	66	NRQ	CA2-C2-N3	9.58	108.20	103.40
1	A	66	NRQ	CA2-C2-N3	9.88	108.35	103.40
3	E	66	NRQ	CA2-C2-N3	10.69	108.76	103.40
3	D	66	NRQ	CA2-C2-N3	10.96	108.89	103.40
3	H	66	NRQ	CA2-C2-N3	11.90	109.37	103.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	66	NRQ	1	0
3	G	66	NRQ	4	0
3	H	66	NRQ	1	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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	216/218 (99%)	0.02	4 (1%) 70 69	28, 40, 48, 53	0
2	B	217/218 (99%)	-0.31	2 (0%) 85 85	27, 38, 47, 53	0
3	C	217/218 (99%)	-0.18	4 (1%) 71 71	28, 40, 48, 66	0
3	D	217/218 (99%)	-0.22	3 (1%) 78 77	26, 35, 43, 51	0
3	E	216/218 (99%)	0.06	4 (1%) 70 69	31, 47, 56, 60	0
3	F	217/218 (99%)	-0.13	4 (1%) 71 71	29, 37, 47, 55	0
3	G	217/218 (99%)	0.88	24 (11%) 7 7	41, 57, 65, 72	0
3	H	217/218 (99%)	-0.04	4 (1%) 71 71	31, 43, 56, 62	0
All	All	1734/1744 (99%)	0.01	49 (2%) 56 55	26, 41, 59, 72	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	169	GLY	6.6
3	F	169	GLY	4.7
3	G	170	GLY	4.4
3	G	168	LYS	4.0
3	E	114	GLN	4.0
3	H	168	LYS	3.7
3	G	219	ALA	3.5
3	G	114	GLN	3.5
1	A	169	GLY	3.4
3	G	7	VAL	3.4
3	D	168	LYS	3.1
3	C	169	GLY	3.1
3	H	170	GLY	3.0
3	F	168	LYS	2.9
1	A	168	LYS	2.9
3	G	49	THR	2.9

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Mol	Chain	Res	Type	RSRZ
3	G	105	VAL	2.9
3	G	225	LEU	2.8
3	H	169	GLY	2.8
3	G	113	LEU	2.7
3	G	17	HIS	2.7
3	G	115	ASP	2.7
3	G	60	ILE	2.6
3	D	6	ASN	2.6
3	G	116	GLY	2.5
3	G	8	ILE	2.5
3	E	168	LYS	2.5
2	B	169	GLY	2.4
3	F	170	GLY	2.4
3	C	168	LYS	2.4
3	G	6	ASN	2.3
1	A	63	PRO	2.3
2	B	168	LYS	2.3
3	G	205	ASN	2.3
3	G	177	PHE	2.2
1	A	206	GLU	2.2
3	G	47	GLN	2.2
3	G	208	TYR	2.2
3	G	210	VAL	2.2
3	G	37	PRO	2.2
3	F	186	PRO	2.2
3	C	6	ASN	2.1
3	G	88	PRO	2.1
3	H	75	HIS	2.1
3	G	191	GLY	2.1
3	G	38	TYR	2.1
3	D	114	GLN	2.0
3	C	170	GLY	2.0
3	E	96	VAL	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NRQ	H	66	23/24	0.94	0.15	-	40,44,47,48	0
3	NRQ	G	66	23/24	0.82	0.25	-	59,60,62,66	0
2	NRQ	B	66	23/24	0.95	0.15	-	38,41,42,46	0
1	NRQ	A	66	23/24	0.95	0.22	-	37,41,43,44	0
3	NRQ	D	66	23/24	0.95	0.16	-	29,34,36,39	0
3	NRQ	C	66	23/24	0.95	0.14	-	35,40,43,44	0
3	NRQ	F	66	23/24	0.96	0.16	-	33,37,39,39	0
3	NRQ	E	66	23/24	0.94	0.14	-	39,44,48,49	0

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.