Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 03:55 PM JST

PDB ID	:	7DNA
Title	:	Photocleavable Fluorescent Protein in green and red form
Authors	:	Wen, Y.; Lemieux, J.M.
Deposited on	:	2020-12-09
Resolution	:	2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

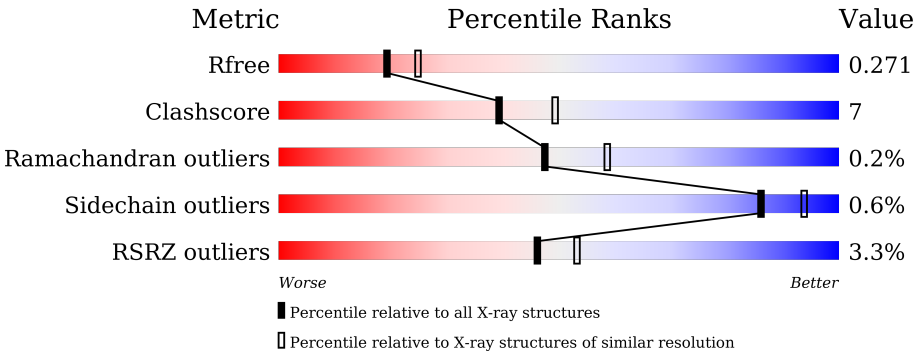
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	240	77% 11% • 11%
1	B	240	.% 73% 15% • 11%
1	D	240	5% 75% 12% 12%
1	K	240	.% 78% 10% • 11%
2	F	240	2% 70% 15% • 15%
2	I	240	7% 75% 12% 13%

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	IEY	F	232	X	-	-	-
2	IEY	I	232	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10676 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.

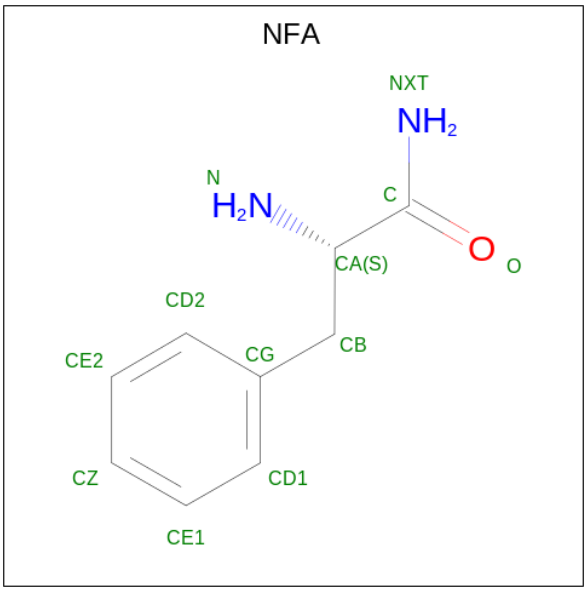
- Molecule 1 is a protein called Green-to-red photoconvertible GFP-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	1	3	0
			1741	1116	296	320	9			
1	B	214	Total	C	N	O	S	1	2	0
			1744	1117	297	321	9			
1	D	210	Total	C	N	O	S	1	2	0
			1708	1093	291	315	9			
1	K	213	Total	C	N	O	S	2	3	0
			1738	1114	296	319	9			

- Molecule 2 is a protein called Green-to-red photoconvertible GFP-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	205	Total	C	N	O	S	1	3	0
			1678	1072	285	312	9			
2	I	208	Total	C	N	O	S	1	2	0
			1694	1084	289	312	9			

- Molecule 3 is PHENYLALANINE AMIDE (three-letter code: NFA) (formula: $C_9H_{12}N_2O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total C N O 12 9 2 1	0	0
3	I	1	Total C N O 12 9 2 1	0	0

- Molecule 4 is water.

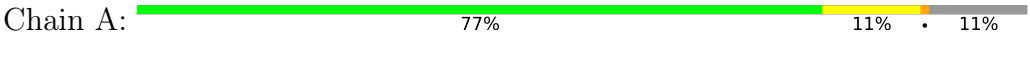
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	64	Total O 64 64	0	0
4	B	57	Total O 57 57	0	0
4	D	68	Total O 68 68	0	0
4	F	61	Total O 61 61	0	0
4	I	51	Total O 51 51	0	0
4	K	48	Total O 48 48	0	0

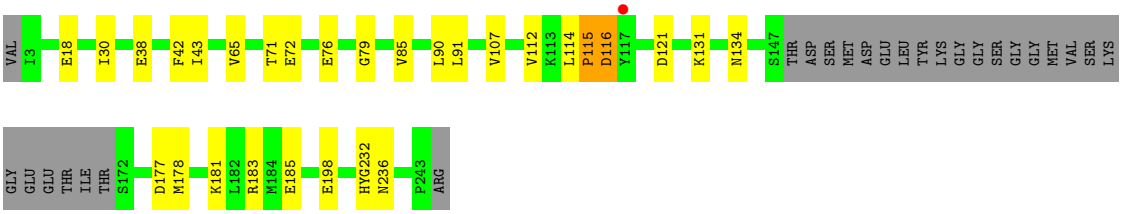
3 Residue-property plots (i)

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

• Molecule 1: Green-to-red photoconvertible GFP-like protein

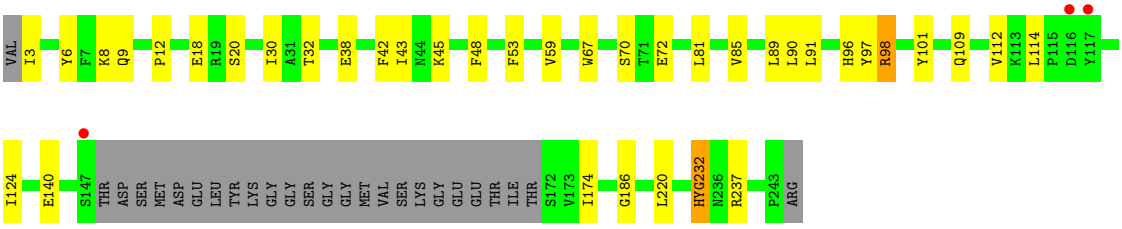
Chain A:





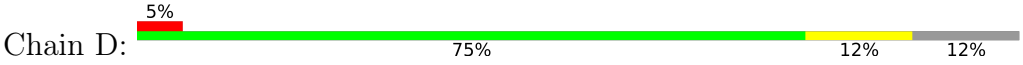
• Molecule 1: Green-to-red photoconvertible GFP-like protein

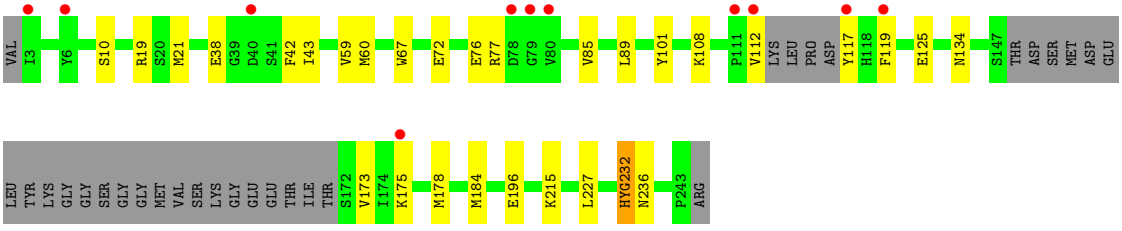
Chain B:



• Molecule 1: Green-to-red photoconvertible GFP-like protein

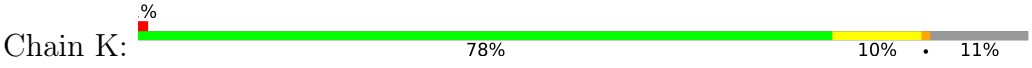
Chain D:

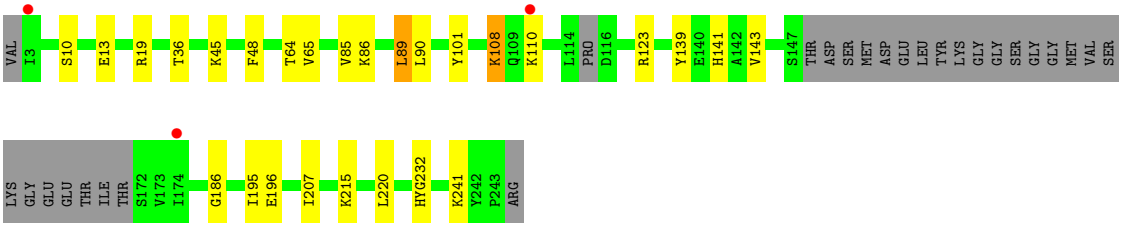




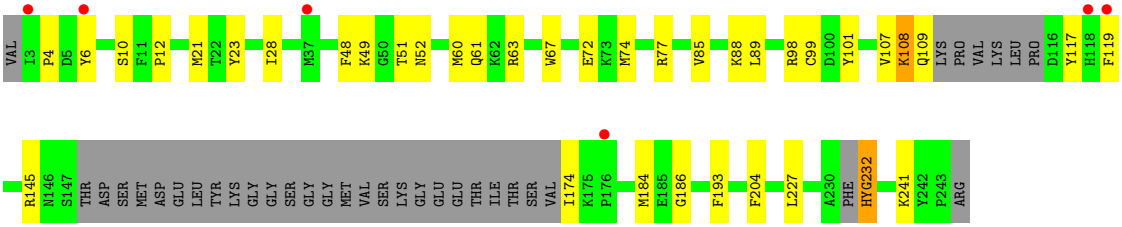
• Molecule 1: Green-to-red photoconvertible GFP-like protein

Chain K:

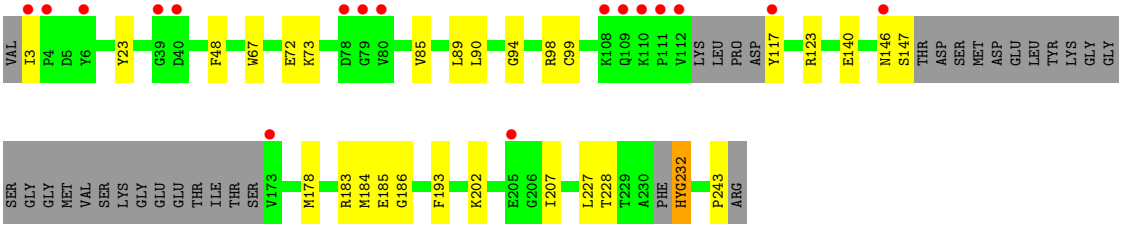




• Molecule 2: Green-to-red photoconvertible GFP-like protein



• Molecule 2: Green-to-red photoconvertible GFP-like protein



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	38.93Å 72.49Å 126.55Å 92.46° 97.31° 92.50°	Depositor
Resolution (Å)	46.27 – 2.30 46.27 – 2.30	Depositor EDS
% Data completeness (in resolution range)	76.4 (46.27-2.30) 76.5 (46.27-2.30)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.94 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.221 , 0.271 0.221 , 0.271	Depositor DCC
R_{free} test set	1992 reflections (4.28%)	wwPDB-VP
Wilson B-factor (Å^2)	23.4	Xtriage
Anisotropy	0.627	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 38.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.068 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	10676	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IEY, CR8, NFA

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	0.31	0/1762	0.57	2/2373 (0.1%)
1	B	0.32	0/1762	0.54	0/2371
1	D	0.31	0/1724	0.53	0/2319
1	K	0.32	0/1757	0.54	1/2362 (0.0%)
2	F	0.29	0/1699	0.53	0/2284
2	I	0.31	0/1710	0.53	0/2299
All	All	0.31	0/10414	0.54	3/14008 (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
2	F	1	0
2	I	1	0
All	All	2	0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	115	PRO	C-N-CA	6.61	138.22	121.70
1	K	89	LEU	CA-CB-CG	6.08	129.29	115.30
1	A	115	PRO	CA-C-N	5.23	128.70	117.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	232	IEY	CA2

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Mol	Chain	Res	Type	Atom
2	I	232	IEY	CA2

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	1741	0	1678	28	0
1	B	1744	0	1684	36	0
1	D	1708	0	1637	20	0
1	K	1738	0	1681	18	0
2	F	1678	0	1621	31	0
2	I	1694	0	1640	22	0
3	F	12	0	10	3	0
3	I	12	0	10	3	0
4	A	64	0	0	4	0
4	B	57	0	0	18	0
4	D	68	0	0	5	0
4	F	61	0	0	6	0
4	I	51	0	0	3	0
4	K	48	0	0	5	0
All	All	10676	0	9961	150	0

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

All (150) 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:A:65:VAL:CG2	1:A:90:LEU:HD12	1.92	0.99
1:B:109:GLN:NE2	4:B:401:HOH:O	1.98	0.97
1:D:38:GLU:OE2	4:D:401:HOH:O	1.84	0.95
1:B:38:GLU:HG2	1:B:43:ILE:HD11	1.60	0.82
1:B:90:LEU:N	4:B:404:HOH:O	2.12	0.82
2:F:232:IEY:HA1	3:F:301:NFA:NXT	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:VAL:HG23	1:A:90:LEU:HD12	1.64	0.78
1:A:90:LEU:HD11	2:I:90:LEU:HD21	1.64	0.77
1:D:173:VAL:O	1:D:175[A]:LYS:NZ	2.19	0.76
2:F:88:LYS:NZ	4:F:402:HOH:O	2.19	0.75
1:B:91:LEU:HD11	1:B:97:TYR:HB2	1.65	0.75
1:B:12:PRO:O	4:B:402:HOH:O	2.06	0.74
1:D:196:GLU:HG3	1:D:215:LYS:HG3	1.70	0.74
1:K:65:VAL:O	4:K:401:HOH:O	2.06	0.73
1:A:177:ASP:O	1:A:178:MET:HE2	1.88	0.73
1:K:64:THR:HB	1:K:89:LEU:HD11	1.71	0.71
1:D:38:GLU:HG2	1:D:43:ILE:HD13	1.73	0.69
1:B:89:LEU:C	4:B:404:HOH:O	2.31	0.69
1:D:125:GLU:OE2	4:D:402:HOH:O	2.12	0.67
1:D:134:ASN:OD1	4:D:403:HOH:O	2.12	0.67
1:B:53:PHE:CD1	1:B:59:VAL:HG21	2.30	0.67
1:D:10:SER:HA	1:D:108:LYS:HG2	1.77	0.66
1:A:134:ASN:OD1	4:A:402:HOH:O	2.14	0.66
2:I:183:ARG:NH1	2:I:185:GLU:OE2	2.29	0.65
1:K:10:SER:HA	1:K:108:LYS:HB2	1.78	0.65
1:B:3:ILE:N	4:B:411:HOH:O	2.31	0.63
1:A:42:PHE:CE2	1:A:178:MET:HG2	2.35	0.61
1:A:90:LEU:HD13	1:A:91:LEU:N	2.15	0.61
2:F:232:IEY:HA1	3:F:301:NFA:HXT2	1.63	0.61
2:F:51:THR:HG23	2:F:52:ASN:HD22	1.66	0.61
2:I:117:TYR:N	4:I:402:HOH:O	2.33	0.60
2:I:202:LYS:HD2	2:I:207:ILE:HD11	1.82	0.60
1:A:65:VAL:HG21	1:A:90:LEU:HD12	1.81	0.59
2:F:12:PRO:HB2	4:F:425:HOH:O	2.03	0.59
1:D:76:GLU:HG3	1:D:112:VAL:HB	1.85	0.59
1:D:42:PHE:CE2	1:D:178:MET:HG2	2.38	0.58
1:K:196:GLU:HB2	1:K:215:LYS:HE3	1.85	0.58
2:F:98:ARG:NH1	4:F:401:HOH:O	2.10	0.58
1:A:30:ILE:HD11	2:F:28:ILE:HG22	1.86	0.58
1:A:183:ARG:NH1	1:A:185:GLU:OE2	2.32	0.58
2:F:204:PHE:O	2:F:241:LYS:HG3	2.05	0.57
2:F:61[A]:GLN:OE1	2:F:63:ARG:NH1	2.38	0.57
2:I:73:LYS:NZ	4:I:403:HOH:O	2.34	0.56
1:A:18:GLU:OE1	4:A:403:HOH:O	2.18	0.56
1:B:18:GLU:HG2	1:B:32:THR:HG22	1.89	0.55
2:I:140:GLU:HB2	2:I:232:IEY:CD3	2.36	0.55
2:I:232:IEY:HA1	3:I:301:NFA:NXT	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:77:ARG:HG3	2:F:77:ARG:HH11	1.71	0.54
1:B:81:LEU:N	4:B:407:HOH:O	2.20	0.54
1:D:19:ARG:HD2	4:D:408:HOH:O	2.07	0.54
1:B:59:VAL:HG22	4:B:437:HOH:O	2.08	0.54
2:I:184:MET:HE2	2:I:193:PHE:HE2	1.73	0.54
1:K:64:THR:HB	1:K:89:LEU:CD1	2.36	0.53
1:A:114:LEU:HB3	1:A:116:ASP:O	2.09	0.53
1:B:81:LEU:HB2	1:B:112:VAL:HG21	1.90	0.53
1:K:13:GLU:OE1	1:K:13:GLU:N	2.39	0.53
1:A:18:GLU:HB2	2:F:51:THR:OG1	2.08	0.52
2:I:3:ILE:HD11	2:I:243:PRO:HD2	1.91	0.52
1:A:71:THR:HG22	1:A:121:ASP:OD1	2.08	0.52
1:D:236:ASN:HB3	4:D:422:HOH:O	2.10	0.52
1:B:8:LYS:NZ	4:B:414:HOH:O	2.41	0.51
1:B:45:LYS:HG3	4:B:422:HOH:O	2.09	0.51
2:F:232:IEY:HD2	2:F:232:IEY:N2	2.25	0.51
2:F:4:PRO:HB2	2:F:6:TYR:CE2	2.46	0.51
1:A:181:LYS:HE3	1:A:198:GLU:HG2	1.93	0.50
1:B:124:ILE:O	4:B:406:HOH:O	2.19	0.49
1:B:53:PHE:CG	1:B:59:VAL:HG21	2.47	0.49
2:F:107:VAL:C	2:F:109:GLN:H	2.14	0.49
2:F:184:MET:HE2	2:F:193:PHE:HE2	1.77	0.49
2:I:23:TYR:CD2	2:I:99:CYS:HB2	2.47	0.49
1:B:85:VAL:HG13	1:B:101:TYR:HB2	1.94	0.48
1:B:237:ARG:NE	1:B:237:ARG:HA	2.27	0.48
1:D:72:GLU:HA	1:D:85:VAL:HB	1.94	0.48
2:F:72:GLU:HA	2:F:85:VAL:HB	1.95	0.48
1:A:107:VAL:HB	4:A:401:HOH:O	2.13	0.48
2:F:23:TYR:CD2	2:F:99:CYS:HB2	2.48	0.48
1:K:86:LYS:NZ	4:K:410:HOH:O	2.38	0.47
1:D:232:CR8:N2	1:D:232:CR8:H5	2.29	0.47
2:I:3:ILE:HG23	2:I:146:ASN:HD21	1.79	0.47
2:I:232:IEY:N21	3:I:301:NFA:NXT	2.62	0.47
1:B:98:ARG:NH2	4:B:419:HOH:O	2.48	0.47
1:B:114:LEU:HD22	4:B:428:HOH:O	2.15	0.47
2:F:174:ILE:N	4:F:412:HOH:O	2.47	0.47
1:K:36:THR:OG1	4:K:402:HOH:O	2.20	0.47
1:A:236:ASN:N	4:A:415:HOH:O	2.48	0.46
2:F:77:ARG:HG3	2:F:77:ARG:NH1	2.31	0.46
1:A:38:GLU:HB2	1:A:43:ILE:HD11	1.97	0.46
1:B:72:GLU:HA	1:B:85:VAL:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:GLU:OE2	1:B:237:ARG:NH2	2.49	0.46
2:F:49:LYS:NZ	4:F:415:HOH:O	2.49	0.46
2:F:184:MET:HE1	2:F:227:LEU:HD22	1.98	0.46
1:B:6:TYR:HA	1:B:9:GLN:HG2	1.98	0.45
2:F:232:IEY:CA1	3:F:301:NFA:NXT	2.76	0.45
2:I:67:TRP:CD2	2:I:89:LEU:HD13	2.51	0.45
1:A:90:LEU:HD21	2:I:94:GLY:HA2	1.99	0.45
1:K:143:VAL:HG23	1:K:241:LYS:HB3	1.99	0.45
1:A:76:GLU:HB2	1:A:114:LEU:HD12	1.98	0.45
2:F:85:VAL:HG13	2:F:101:TYR:HB2	1.99	0.45
2:I:184:MET:HE1	2:I:227:LEU:HD22	1.97	0.45
1:B:232:CR8:N2	1:B:232:CR8:H5	2.32	0.45
1:B:42:PHE:HZ	1:B:174:ILE:HD12	1.82	0.44
2:I:48:PHE:O	2:I:186:GLY:HA2	2.17	0.44
1:B:6:TYR:HE2	1:B:114:LEU:HD21	1.83	0.44
2:F:108:LYS:O	2:F:108:LYS:HG2	2.18	0.43
1:B:70:SER:HB3	4:B:410:HOH:O	2.17	0.43
1:B:237:ARG:NH2	4:B:420:HOH:O	2.50	0.43
2:F:48:PHE:O	2:F:186:GLY:HA2	2.18	0.43
1:B:48:PHE:O	1:B:186:GLY:HA2	2.18	0.43
1:D:59:VAL:HG12	1:D:60:MET:HE2	2.01	0.43
2:F:67:TRP:CD2	2:F:89:LEU:HD13	2.54	0.43
2:F:119:PHE:HB2	2:F:145:ARG:HG3	2.01	0.43
2:I:232:IEY:HD2	2:I:232:IEY:N2	2.34	0.43
1:B:67:TRP:CZ3	1:B:89:LEU:HG	2.54	0.43
2:F:21:MET:HG2	2:F:101:TYR:CE1	2.54	0.43
2:I:72:GLU:HA	2:I:85:VAL:HB	2.00	0.43
1:D:21:MET:HG2	1:D:101:TYR:CE1	2.54	0.43
1:K:19:ARG:HD2	4:K:423:HOH:O	2.19	0.42
1:K:48:PHE:O	1:K:186:GLY:HA2	2.20	0.42
1:A:90:LEU:HD13	1:A:91:LEU:O	2.19	0.42
1:A:79:GLY:HA2	1:A:112:VAL:O	2.19	0.42
1:B:96:HIS:HD2	4:B:404:HOH:O	2.02	0.42
2:I:228:THR:HA	3:I:301:NFA:HD2	2.02	0.42
1:D:117:TYR:CE2	1:D:119:PHE:HE1	2.38	0.41
1:K:85:VAL:HG13	1:K:101:TYR:HB2	2.01	0.41
1:K:195:ILE:HD11	1:K:220:LEU:HD11	2.02	0.41
1:K:13:GLU:CD	1:K:108:LYS:HE3	2.41	0.41
1:K:123:ARG:HB2	1:K:141:HIS:HB3	2.02	0.41
1:A:76:GLU:HG3	1:A:112:VAL:HG23	2.02	0.41
2:F:60:MET:HG2	4:F:417:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:45:LYS:HE2	4:K:402:HOH:O	2.20	0.41
1:A:90:LEU:CD1	2:I:90:LEU:HD21	2.43	0.41
1:B:140:GLU:CD	1:B:237:ARG:HH22	2.24	0.41
1:D:67:TRP:CD2	1:D:89:LEU:HD13	2.55	0.41
2:F:74:MET:O	2:F:117:TYR:HB2	2.21	0.41
1:K:65:VAL:HG23	1:K:90:LEU:HB3	2.02	0.41
1:B:20:SER:HA	1:B:30:ILE:HD13	2.03	0.41
1:A:72:GLU:HB2	1:A:85:VAL:HB	2.02	0.41
1:D:184:MET:HE1	1:D:227:LEU:HD22	2.03	0.41
1:B:98:ARG:NH2	4:B:409:HOH:O	2.29	0.41
2:F:6:TYR:O	2:F:10:SER:OG	2.39	0.41
2:I:98:ARG:HG2	4:I:436:HOH:O	2.20	0.41
1:B:220:LEU:HG	4:B:405:HOH:O	2.20	0.41
1:K:139:TYR:CE1	1:K:207:ILE:HG23	2.55	0.41
1:B:96:HIS:O	4:B:408:HOH:O	2.22	0.40
1:A:115:PRO:HB2	1:A:116:ASP:CB	2.51	0.40
1:D:196:GLU:HG3	1:D:215:LYS:CG	2.47	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	208/240 (87%)	202 (97%)	5 (2%)	1 (0%)	29 35
1	B	207/240 (86%)	204 (99%)	3 (1%)	0	100 100
1	D	201/240 (84%)	194 (96%)	7 (4%)	0	100 100
1	K	205/240 (85%)	198 (97%)	7 (3%)	0	100 100
2	F	198/240 (82%)	192 (97%)	5 (2%)	1 (0%)	29 35
2	I	199/240 (83%)	195 (98%)	4 (2%)	0	100 100
All	All	1218/1440 (85%)	1185 (97%)	31 (2%)	2 (0%)	47 58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	ASP
2	F	108	LYS

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	185/207 (89%)	184 (100%)	1 (0%)	88 95
1	B	186/207 (90%)	185 (100%)	1 (0%)	88 95
1	D	181/207 (87%)	180 (99%)	1 (1%)	86 94
1	K	185/207 (89%)	183 (99%)	2 (1%)	73 86
2	F	178/207 (86%)	178 (100%)	0	100 100
2	I	180/207 (87%)	178 (99%)	2 (1%)	73 86
All	All	1095/1242 (88%)	1088 (99%)	7 (1%)	86 94

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	131	LYS
1	B	98	ARG
1	D	77	ARG
2	I	123	ARG
2	I	147	SER
1	K	108	LYS
1	K	110	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	208	GLN
1	B	52	ASN
1	B	96	HIS

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Mol	Chain	Res	Type
1	B	208	GLN
2	F	52	ASN
2	F	146	ASN
2	I	146	ASN
1	K	9	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

6 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	CR8	A	232	1	20,27,28	2.10	11 (55%)	17,37,39	1.54	2 (11%)
2	IEY	I	232	2	24,26,27	5.78	8 (33%)	24,35,37	3.54	5 (20%)
2	IEY	F	232	2	24,26,27	5.57	8 (33%)	24,35,37	3.40	7 (29%)
1	CR8	B	232	1	20,27,28	2.10	11 (55%)	17,37,39	1.68	2 (11%)
1	CR8	D	232	1	20,27,28	2.11	9 (45%)	17,37,39	1.73	2 (11%)
1	CR8	K	232	1	20,27,28	2.06	10 (50%)	17,37,39	1.56	2 (11%)

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	IEY	I	232	2	1/1/4/7	5/9/28/29	0/3/3/3
2	IEY	F	232	2	1/1/4/7	4/9/28/29	0/3/3/3
1	CR8	B	232	1	-	2/8/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CR8	K	232	1	-	5/8/25/26	0/3/3/3
1	CR8	D	232	1	-	4/8/25/26	0/3/3/3
1	CR8	A	232	1	-	5/8/25/26	0/3/3/3

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	232	IEY	CA2-C2	-22.39	1.36	1.52
2	F	232	IEY	CA2-C2	-21.15	1.37	1.52
2	F	232	IEY	O2-C2	10.41	1.40	1.22
2	I	232	IEY	O2-C2	10.27	1.40	1.22
2	F	232	IEY	CA2-N2	-10.12	1.31	1.47
2	I	232	IEY	CA2-N2	-9.64	1.32	1.47
2	I	232	IEY	CA1-C1	6.17	1.53	1.45
2	F	232	IEY	CA1-C1	5.48	1.52	1.45
2	I	232	IEY	C2-N3	-5.47	1.30	1.38
2	F	232	IEY	C2-N3	-5.13	1.31	1.38
1	B	232	CR8	C2-N3	-3.63	1.30	1.36
1	K	232	CR8	C2-N3	-3.51	1.30	1.36
1	D	232	CR8	CA2-C8	3.50	1.54	1.41
1	D	232	CR8	C2-N3	-3.49	1.30	1.36
1	B	232	CR8	CA2-C8	3.47	1.54	1.41
1	A	232	CR8	CA2-C8	3.47	1.54	1.41
1	K	232	CR8	CA2-C8	3.43	1.54	1.41
1	A	232	CR8	C2-N3	-3.41	1.30	1.36
1	D	232	CR8	C1-CA1	3.26	1.55	1.50
1	A	232	CR8	C1-CA1	3.18	1.55	1.50
1	A	232	CR8	O2-C2	3.17	1.42	1.32
1	B	232	CR8	O2-C2	3.15	1.41	1.32
1	D	232	CR8	O2-C2	3.09	1.41	1.32
1	K	232	CR8	O2-C2	3.06	1.41	1.32
2	I	232	IEY	CG1-N21	-2.97	1.28	1.37
1	B	232	CR8	C1-CA1	2.92	1.55	1.50
2	F	232	IEY	CG1-N21	-2.85	1.28	1.37
2	I	232	IEY	C1-N3	-2.76	1.34	1.38
1	K	232	CR8	C1-CA1	2.73	1.54	1.50
2	F	232	IEY	CG1-CB1	2.70	1.53	1.47
2	I	232	IEY	CG1-CB1	2.67	1.53	1.47
1	B	232	CR8	C12-C11	-2.64	1.39	1.45
1	A	232	CR8	C12-C11	-2.61	1.40	1.45
2	F	232	IEY	C1-N3	-2.54	1.34	1.38
1	K	232	CR8	C12-C11	-2.52	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	232	CR8	C12-C11	-2.40	1.40	1.45
1	D	232	CR8	CA3-N3	-2.39	1.45	1.49
1	D	232	CR8	C6-C12	2.38	1.40	1.35
1	B	232	CR8	CA3-N3	-2.32	1.45	1.49
1	K	232	CR8	CA3-N3	-2.31	1.45	1.49
1	D	232	CR8	C5-C4	2.30	1.40	1.35
1	A	232	CR8	CA3-N3	-2.28	1.45	1.49
1	K	232	CR8	C6-C12	2.27	1.40	1.35
1	B	232	CR8	C5-C4	2.25	1.40	1.35
1	A	232	CR8	C6-C12	2.25	1.40	1.35
1	D	232	CR8	CA1-N1	-2.24	1.42	1.47
1	K	232	CR8	C5-C4	2.17	1.40	1.35
1	K	232	CR8	CA1-N1	-2.16	1.42	1.47
1	A	232	CR8	C5-C4	2.15	1.40	1.35
1	B	232	CR8	C6-C12	2.08	1.40	1.35
1	B	232	CR8	C1-N2	2.07	1.37	1.34
1	K	232	CR8	C20-C21	2.06	1.58	1.51
1	A	232	CR8	C1-N2	2.05	1.37	1.34
1	A	232	CR8	C4-C11	-2.04	1.41	1.45
1	B	232	CR8	C20-C21	2.03	1.58	1.51
1	B	232	CR8	CA1-N1	-2.01	1.42	1.47
1	A	232	CR8	C20-C21	2.00	1.58	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	232	IEY	CB2-CA2-N2	15.30	130.94	110.78
2	F	232	IEY	CB2-CA2-N2	13.41	128.45	110.78
2	F	232	IEY	CB2-CA2-C2	5.82	123.99	110.49
1	D	232	CR8	C3-CA3-N3	5.17	119.76	111.92
2	I	232	IEY	CB2-CA2-C2	4.76	121.53	110.49
1	B	232	CR8	C3-CA3-N3	4.47	118.70	111.92
1	A	232	CR8	C3-CA3-N3	4.22	118.31	111.92
2	F	232	IEY	CG1-CB1-CA1	-3.83	116.97	126.14
1	K	232	CR8	C3-CA3-N3	3.64	117.44	111.92
2	I	232	IEY	CG2-CB2-CA2	3.39	120.22	113.40
2	F	232	IEY	CB1-CA1-C1	3.20	127.94	122.90
2	F	232	IEY	CA3-N3-C2	2.96	126.12	123.43
2	F	232	IEY	CG2-CB2-CA2	2.73	118.88	113.40
1	A	232	CR8	O3-C3-CA3	-2.72	118.60	126.32
1	B	232	CR8	O3-C3-CA3	-2.60	118.94	126.32
1	D	232	CR8	O3-C3-CA3	-2.55	119.06	126.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	232	CR8	O3-C3-CA3	-2.44	119.39	126.32
2	F	232	IEY	O3-C3-CA3	-2.39	119.19	126.39
2	I	232	IEY	O3-C3-CA3	-2.18	119.82	126.39
2	I	232	IEY	CB2-CG2-CD1	-2.12	116.69	120.91

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	232	IEY	CA2
2	I	232	IEY	CA2

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	232	CR8	C7-C8-CA2-C2
1	A	232	CR8	C7-C8-CA2-N2
1	A	232	CR8	CA1-C20-C21-N22
1	A	232	CR8	CA1-C20-C21-C23
1	B	232	CR8	CA1-C20-C21-N22
1	B	232	CR8	CA1-C20-C21-C23
1	D	232	CR8	C7-C8-CA2-N2
1	D	232	CR8	CA1-C20-C21-N22
1	D	232	CR8	CA1-C20-C21-C23
1	K	232	CR8	C7-C8-CA2-C2
1	K	232	CR8	C7-C8-CA2-N2
1	K	232	CR8	CA1-C20-C21-N22
1	K	232	CR8	CA1-C20-C21-C23
2	F	232	IEY	N2-CA2-CB2-CG2
2	I	232	IEY	N2-CA2-CB2-CG2
2	I	232	IEY	CA2-CB2-CG2-CD2
2	I	232	IEY	CA2-CB2-CG2-CD1
1	D	232	CR8	C21-C20-CA1-N1
2	F	232	IEY	CA2-CB2-CG2-CD1
2	F	232	IEY	CA2-CB2-CG2-CD2
1	A	232	CR8	C21-C20-CA1-N1
1	K	232	CR8	C21-C20-CA1-N1
2	I	232	IEY	C3-CA3-N3-C2
2	F	232	IEY	C2-CA2-CB2-CG2
2	I	232	IEY	C2-CA2-CB2-CG2

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	232	IEY	4	0
2	F	232	IEY	4	0
1	B	232	CR8	1	0
1	D	232	CR8	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
3	NFA	F	301	2	12,12,12	1.41	2 (16%)	15,15,15	1.13	2 (13%)
3	NFA	I	301	2	12,12,12	1.50	2 (16%)	15,15,15	1.06	2 (13%)

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
3	NFA	F	301	2	-	6/8/8/8	0/1/1/1
3	NFA	I	301	2	-	5/8/8/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	301	NFA	C-NXT	4.26	1.43	1.32
3	F	301	NFA	C-NXT	4.04	1.43	1.32
3	I	301	NFA	O-C	-2.78	1.18	1.23
3	F	301	NFA	O-C	-2.55	1.19	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	301	NFA	O-C-NXT	-2.69	118.33	123.00
3	I	301	NFA	O-C-NXT	-2.40	118.83	123.00
3	I	301	NFA	CG-CB-CA	-2.35	109.25	114.13
3	F	301	NFA	CG-CB-CA	-2.20	109.56	114.13

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	301	NFA	NXT-C-CA-N
3	I	301	NFA	O-C-CA-N
3	I	301	NFA	O-C-CA-CB
3	I	301	NFA	NXT-C-CA-CB
3	F	301	NFA	O-C-CA-N
3	I	301	NFA	N-CA-CB-CG
3	F	301	NFA	O-C-CA-CB
3	F	301	NFA	CA-CB-CG-CD1
3	F	301	NFA	NXT-C-CA-CB
3	F	301	NFA	CA-CB-CG-CD2
3	I	301	NFA	CA-CB-CG-CD1

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	301	NFA	3	0
3	I	301	NFA	3	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	213/240 (88%)	-0.08	1 (0%)	91	94	11, 22, 43, 58	1 (0%)
1	B	213/240 (88%)	0.04	3 (1%)	75	80	12, 26, 46, 60	1 (0%)
1	D	209/240 (87%)	0.30	11 (5%)	26	33	10, 28, 59, 77	1 (0%)
1	K	212/240 (88%)	0.21	3 (1%)	75	80	18, 31, 54, 62	2 (0%)
2	F	204/240 (85%)	0.19	6 (2%)	51	58	10, 28, 53, 64	2 (0%)
2	I	207/240 (86%)	0.24	17 (8%)	11	15	12, 28, 58, 78	2 (0%)
All	All	1258/1440 (87%)	0.15	41 (3%)	46	53	10, 27, 54, 78	9 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	117	TYR	5.4
1	D	112	VAL	4.6
2	I	79	GLY	3.8
1	D	79	GLY	3.7
1	K	174	ILE	3.6
1	K	3	ILE	3.5
2	I	39	GLY	3.5
2	I	173	VAL	3.4
2	I	111	PRO	3.3
1	D	117	TYR	3.3
1	D	119	PHE	3.2
2	F	118	HIS	3.1
2	I	112	VAL	3.0
2	I	78	ASP	3.0
1	A	117	TYR	3.0
2	I	3	ILE	2.9
1	D	3	ILE	2.9
2	I	80	VAL	2.9
1	D	111	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	I	40	ASP	2.8
2	F	119	PHE	2.8
1	K	110	LYS	2.7
2	I	6	TYR	2.7
1	B	117	TYR	2.7
1	D	80	VAL	2.7
1	B	116	ASP	2.6
2	I	205	GLU	2.5
2	F	3	ILE	2.4
2	F	6	TYR	2.4
1	D	175[A]	LYS	2.3
2	F	37	MET	2.3
1	D	78	ASP	2.3
2	I	110	LYS	2.3
1	D	40	ASP	2.2
1	B	147	SER	2.2
2	I	108	LYS	2.1
2	I	146	ASN	2.1
2	I	109	GLN	2.0
1	D	6	TYR	2.0
2	F	176	PRO	2.0
2	I	4	PRO	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. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	IEY	F	232	24/25	0.90	0.17	21,25,37,38	0
2	IEY	I	232	24/25	0.91	0.16	21,27,30,32	0
1	CR8	D	232	25/26	0.93	0.14	19,25,34,36	0
1	CR8	K	232	25/26	0.93	0.14	20,24,30,32	0
1	CR8	B	232	25/26	0.94	0.14	16,21,25,28	0
1	CR8	A	232	25/26	0.96	0.11	14,17,23,30	0

6.3 Carbohydrates (i)

There are no monosaccharides 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. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NFA	F	301	12/12	0.88	0.18	16,18,29,43	0
3	NFA	I	301	12/12	0.90	0.17	20,20,37,44	0

6.5 Other polymers

There are no such residues in this entry.