Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2016 – 08:46 AM EDT

PDB ID	:	5D3E
Title	:	Crystal structure of human 14-3-3 gamma in complex with CFTR R-domain peptide pS768-pS795
Authors	:	Stevers, L.M.; Leysen, S.F.R.; Ottmann, C.
Deposited on	:	2015-08-06
Resolution	:	2.75 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 ⓘ symbol.

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

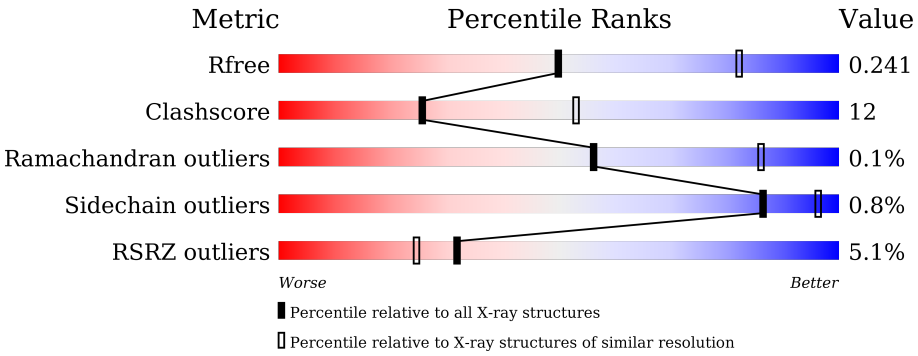
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027107

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 2.75 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.



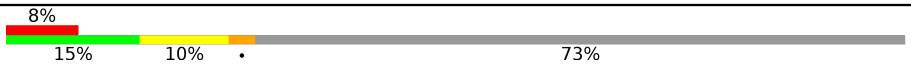
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	241	2% 85% 12% ·
1	B	241	4% 78% 20% ··
1	E	241	2% 77% 20% ·
1	F	241	82% 16% ·
1	I	241	2% 75% 22% ·
1	J	241	20% 58% 35% 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	C	40	
2	G	40	
2	K	40	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11713 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 14-3-3 protein gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	1	0
			1902	1186	324	383	9			
1	B	238	Total	C	N	O	S	0	0	0
			1915	1194	326	384	11			
1	E	234	Total	C	N	O	S	0	2	0
			1900	1186	323	382	9			
1	F	238	Total	C	N	O	S	0	1	0
			1921	1198	326	386	11			
1	I	235	Total	C	N	O	S	0	0	0
			1897	1183	323	382	9			
1	J	224	Total	C	N	O	S	0	0	0
			1814	1135	311	359	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	initiating methionine	UNP P61981
A	-1	GLY	-	expression tag	UNP P61981
A	0	SER	-	expression tag	UNP P61981
B	-2	MET	-	initiating methionine	UNP P61981
B	-1	GLY	-	expression tag	UNP P61981
B	0	SER	-	expression tag	UNP P61981
E	-2	MET	-	initiating methionine	UNP P61981
E	-1	GLY	-	expression tag	UNP P61981
E	0	SER	-	expression tag	UNP P61981
F	-2	MET	-	initiating methionine	UNP P61981
F	-1	GLY	-	expression tag	UNP P61981
F	0	SER	-	expression tag	UNP P61981
I	-2	MET	-	initiating methionine	UNP P61981
I	-1	GLY	-	expression tag	UNP P61981
I	0	SER	-	expression tag	UNP P61981
J	-2	MET	-	initiating methionine	UNP P61981
J	-1	GLY	-	expression tag	UNP P61981

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	0	SER	-	expression tag	UNP P61981

- Molecule 2 is a protein called Cystic fibrosis transmembrane conductance regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	P	0	0	0
			91	53	16	20	2			
2	G	11	Total	C	N	O	P	0	0	0
			88	51	14	21	2			
2	K	5	Total	C	N	O	P	0	0	0
			44	22	6	14	2			

- Molecule 3 is water.

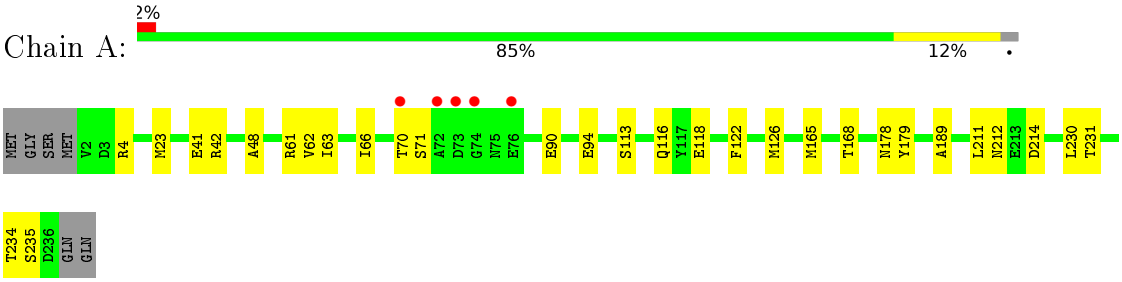
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		
3	B	19	Total	O	0	0
			19	19		
3	C	1	Total	O	0	0
			1	1		
3	E	37	Total	O	0	0
			37	37		
3	F	34	Total	O	0	0
			34	34		
3	G	1	Total	O	0	0
			1	1		
3	I	12	Total	O	0	0
			12	12		
3	J	2	Total	O	0	0
			2	2		
3	K	1	Total	O	0	0
			1	1		

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.

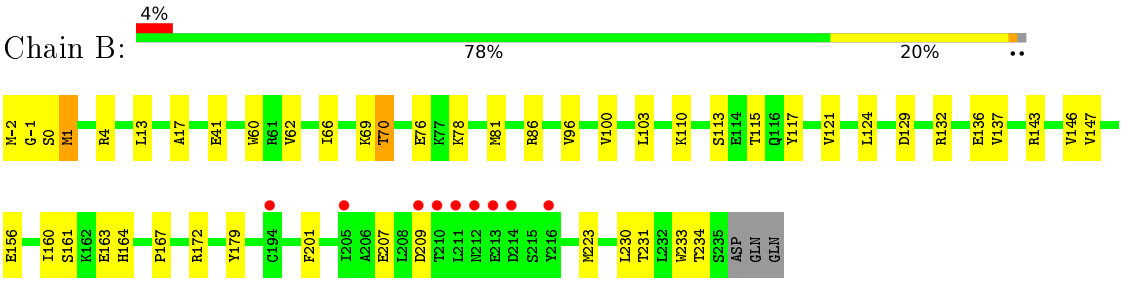
- Molecule 1: 14-3-3 protein gamma

Chain A:



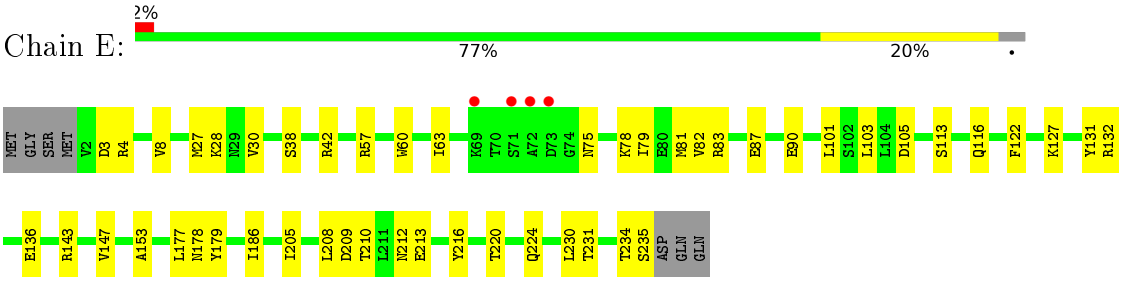
- Molecule 1: 14-3-3 protein gamma

Chain B:



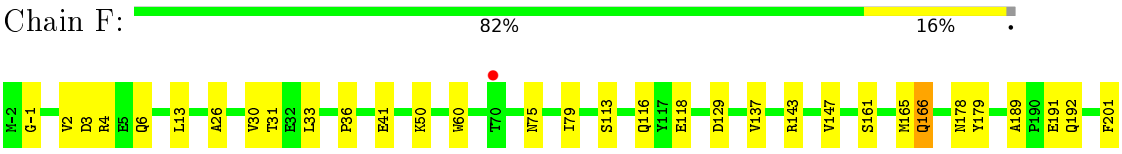
- Molecule 1: 14-3-3 protein gamma

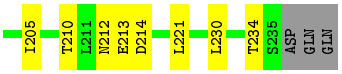
Chain E:



- Molecule 1: 14-3-3 protein gamma

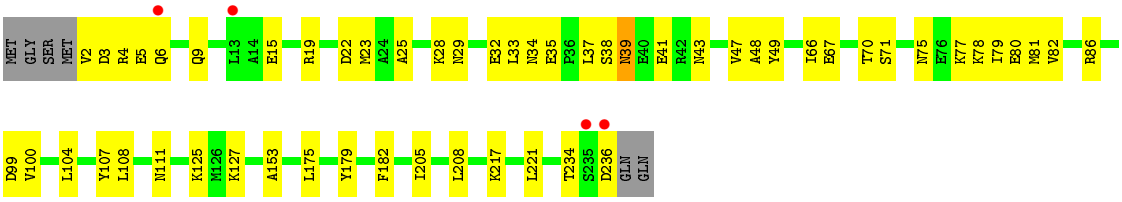
Chain F:





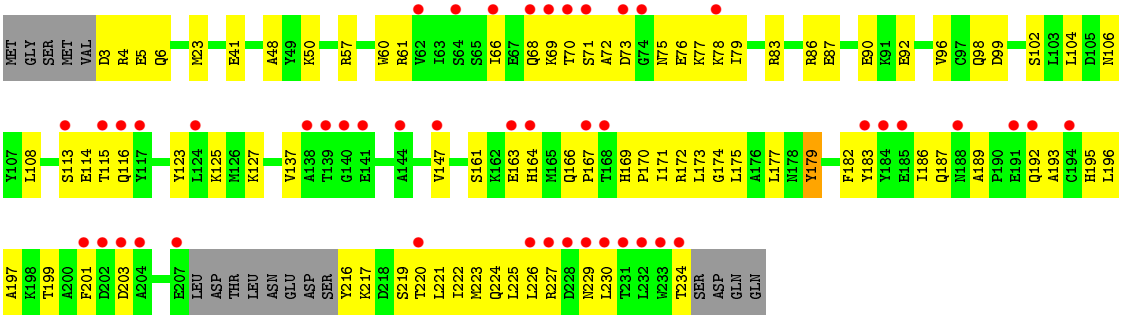
• Molecule 1: 14-3-3 protein gamma

Chain I:



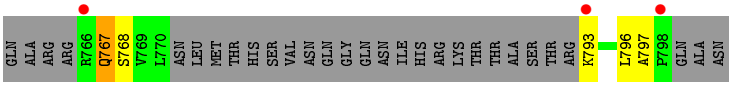
• Molecule 1: 14-3-3 protein gamma

Chain J:



• Molecule 2: Cystic fibrosis transmembrane conductance regulator

Chain C:



• Molecule 2: Cystic fibrosis transmembrane conductance regulator

Chain G:

• Molecule 2: Cystic fibrosis transmembrane conductance regulator

Chain K:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	122.45Å 122.45Å 313.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.30 – 2.75 36.30 – 2.75	Depositor EDS
% Data completeness (in resolution range)	100.0 (36.30-2.75) 98.4 (36.30-2.75)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.36 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.202 , 0.244 0.201 , 0.241	Depositor DCC
R_{free} test set	3002 reflections (4.86%)	DCC
Wilson B-factor (Å^2)	52.4	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 32.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 62806 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11713	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% 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: SEP

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	0.81	0/1934	0.64	1/2610 (0.0%)
1	B	0.64	0/1943	0.56	0/2620
1	E	0.58	0/1935	0.60	0/2612
1	F	0.78	1/1952 (0.1%)	0.65	2/2632 (0.1%)
1	I	0.68	0/1925	0.63	0/2598
1	J	0.47	0/1841	0.57	2/2481 (0.1%)
2	C	0.77	0/68	1.00	1/86 (1.2%)
2	G	0.75	0/65	0.74	0/83
2	K	0.89	0/22	0.70	0/27
All	All	0.67	1/11685 (0.0%)	0.61	6/15749 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	36	PRO	N-CD	5.16	1.55	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	189	ALA	C-N-CD	5.99	140.97	128.40
1	J	75	ASN	N-CA-C	-5.86	95.19	111.00
1	A	189	ALA	C-N-CD	5.81	140.59	128.40
1	J	169	HIS	C-N-CD	5.76	140.49	128.40
1	F	166	GLN	C-N-CD	5.65	140.26	128.40
2	C	767	GLN	N-CA-C	5.50	125.84	111.00

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	1902	0	1867	18	0
1	B	1915	0	1888	41	2
1	E	1900	0	1869	32	0
1	F	1921	0	1894	33	1
1	I	1897	0	1863	60	3
1	J	1814	0	1790	110	6
2	C	91	0	90	3	0
2	G	88	0	83	4	0
2	K	44	0	35	1	0
3	A	34	0	0	2	0
3	B	19	0	0	0	0
3	C	1	0	0	0	0
3	E	37	0	0	0	0
3	F	34	0	0	0	0
3	G	1	0	0	0	0
3	I	12	0	0	0	0
3	J	2	0	0	0	0
3	K	1	0	0	0	0
All	All	11713	0	11379	286	9

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 12.

All (286) 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:J:182:PHE:CE1	1:J:186:ILE:HG21	1.29	1.62
1:J:182:PHE:CE1	1:J:186:ILE:CG2	1.82	1.55
1:J:182:PHE:HE1	1:J:186:ILE:CG2	1.21	1.34
1:J:182:PHE:CD1	1:J:186:ILE:HG21	1.71	1.25
1:J:182:PHE:CD1	1:J:186:ILE:CG2	2.22	1.21
1:B:231:THR:O	1:B:234:THR:HG22	1.37	1.19
1:J:182:PHE:CE1	1:J:186:ILE:HG22	1.73	1.15
1:J:222:ILE:HA	1:J:225:LEU:HD12	1.33	1.10
1:J:182:PHE:CD1	1:J:186:ILE:CB	2.36	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:182:PHE:CD1	1:J:186:ILE:HB	1.90	1.07
1:J:182:PHE:HD1	1:J:186:ILE:CB	1.73	0.98
1:B:66:ILE:O	1:B:70:THR:OG1	1.85	0.94
1:J:70:THR:OG1	1:J:79:ILE:HG12	1.69	0.92
1:F:191:GLU:HG2	1:F:192:GLN:N	1.90	0.85
1:J:182:PHE:O	1:J:186:ILE:HB	1.79	0.82
1:B:-2:MET:HA	1:B:1:MET:HE3	1.60	0.82
1:B:-2:MET:O	1:B:1:MET:HG3	1.79	0.82
1:F:113:SER:H	1:F:116:GLN:NE2	1.78	0.81
1:J:222:ILE:HA	1:J:225:LEU:CD1	2.09	0.81
1:F:191:GLU:HG2	1:F:192:GLN:H	1.45	0.81
1:J:76:GLU:O	1:J:79:ILE:N	2.13	0.81
1:J:147:VAL:HG13	1:J:182:PHE:HZ	1.44	0.80
1:I:2:VAL:HG12	1:I:3:ASP:OD1	1.81	0.80
1:J:170:PRO:HA	1:J:173:LEU:HD12	1.63	0.79
1:J:221:LEU:O	1:J:225:LEU:HG	1.84	0.78
1:J:76:GLU:O	1:J:78:LYS:N	2.17	0.77
1:B:-2:MET:HA	1:B:1:MET:CE	2.13	0.77
1:J:173:LEU:CD1	1:J:219:SER:HB2	2.15	0.77
1:I:2:VAL:HG12	1:I:3:ASP:N	2.00	0.76
1:J:220:THR:O	1:J:223:MET:HB2	1.88	0.74
1:I:2:VAL:CG1	1:I:3:ASP:OD1	2.36	0.73
1:I:81:MET:HE1	1:J:6:GLN:HG2	1.68	0.73
1:J:182:PHE:HD1	1:J:186:ILE:HB	1.41	0.71
1:J:187:GLN:OE1	1:J:187:GLN:HA	1.89	0.71
1:J:147:VAL:HG13	1:J:182:PHE:CZ	2.24	0.71
1:J:76:GLU:O	1:J:77:LYS:C	2.28	0.71
1:I:29:ASN:HA	1:I:32:GLU:HG3	1.72	0.70
1:J:70:THR:CB	1:J:79:ILE:HG12	2.23	0.69
1:F:31:THR:O	1:F:33:LEU:O	2.11	0.69
1:A:230:LEU:O	1:A:234:THR:HG23	1.94	0.68
1:J:86:ARG:NH2	1:J:87:GLU:OE2	2.26	0.68
1:J:114:GLU:HA	1:J:114:GLU:OE1	1.94	0.67
1:B:-2:MET:SD	1:B:1:MET:HE3	2.35	0.67
1:J:102:SER:O	1:J:106:ASN:ND2	2.24	0.67
1:J:4:ARG:NH2	1:J:41:GLU:OE2	2.29	0.66
1:J:217:LYS:HG2	1:J:217:LYS:O	1.96	0.66
1:J:115:THR:HG23	1:J:116:GLN:N	2.10	0.65
1:A:113:SER:N	1:A:116:GLN:OE1	2.18	0.65
1:I:29:ASN:O	1:I:32:GLU:HB2	1.96	0.65
1:J:183:TYR:HA	1:J:187:GLN:HB2	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:220:THR:HA	1:J:223:MET:HG3	1.76	0.65
1:F:201:PHE:CZ	1:F:205:ILE:HD11	2.31	0.65
1:I:3:ASP:O	1:I:6:GLN:N	2.30	0.64
1:I:3:ASP:O	1:I:4:ARG:C	2.34	0.64
1:I:99:ASP:OD1	1:I:100:VAL:N	2.30	0.64
1:J:182:PHE:HD1	1:J:186:ILE:CG1	2.11	0.63
1:J:83:ARG:HA	1:J:86:ARG:HH12	1.63	0.63
1:J:216:TYR:CD1	1:J:217:LYS:HB2	2.35	0.62
1:I:4:ARG:NH2	1:I:35:GLU:HB2	2.15	0.62
1:F:166:GLN:CD	1:F:210:THR:HG21	2.20	0.62
1:F:113:SER:N	1:F:116:GLN:NE2	2.49	0.61
1:A:62:VAL:O	1:A:66:ILE:HG13	2.01	0.61
1:I:32:GLU:HA	1:I:107:TYR:CZ	2.35	0.61
1:E:230:LEU:O	1:E:234:THR:HG22	2.00	0.60
1:I:49:TYR:CD1	1:I:100:VAL:CG1	2.84	0.60
1:J:76:GLU:C	1:J:78:LYS:N	2.46	0.60
1:E:38:SER:HA	1:J:76:GLU:HG3	1.84	0.60
1:J:57:ARG:O	1:J:61:ARG:HD3	2.02	0.59
1:J:216:TYR:O	1:J:217:LYS:HB3	2.02	0.59
1:B:233:TRP:HE1	2:C:793:LYS:HG3	1.67	0.59
1:I:6:GLN:HA	1:I:6:GLN:OE1	2.02	0.59
1:J:71:SER:OG	1:J:72:ALA:N	2.36	0.59
1:I:4:ARG:HH21	1:I:35:GLU:HB2	1.68	0.59
1:J:173:LEU:HD13	1:J:219:SER:HB2	1.84	0.58
1:E:75:ASN:O	1:E:79:ILE:HG13	2.03	0.58
1:J:220:THR:O	1:J:223:MET:N	2.36	0.58
1:E:28:LYS:HG3	1:E:103:LEU:HD11	1.85	0.58
1:F:-1:GLY:O	1:F:2:VAL:O	2.20	0.58
1:I:81:MET:CE	1:J:6:GLN:HE21	2.17	0.58
1:E:210:THR:HG22	1:E:210:THR:O	2.04	0.58
1:F:113:SER:N	1:F:116:GLN:HE21	2.01	0.58
1:B:143:ARG:O	1:B:146:VAL:HG23	2.05	0.57
1:I:49:TYR:CE1	1:I:100:VAL:CG1	2.88	0.57
1:J:66:ILE:O	1:J:70:THR:HG23	2.04	0.57
1:J:68:GLN:O	1:J:71:SER:OG	2.13	0.57
1:A:231:THR:O	1:A:235:SER:HB3	2.05	0.57
1:I:4:ARG:NH2	1:I:35:GLU:CB	2.68	0.56
1:A:23:MET:HG2	1:A:48:ALA:HB2	1.87	0.56
1:E:113:SER:O	1:E:116:GLN:HB2	2.05	0.56
1:A:118:GLU:HG2	1:A:165:MET:HE2	1.87	0.56
1:I:205:ILE:HA	1:I:208:LEU:HD13	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:76:GLU:C	1:J:78:LYS:H	2.08	0.56
1:I:34:ASN:OD1	1:I:111:ASN:ND2	2.38	0.56
1:I:217:LYS:O	1:I:221:LEU:HG	2.06	0.55
1:B:-2:MET:SD	1:B:1:MET:CE	2.94	0.55
1:J:177:LEU:HD13	1:J:226:LEU:HD23	1.87	0.55
1:J:230:LEU:O	1:J:234:THR:HG23	2.07	0.55
1:I:77:LYS:HD2	1:I:80:GLU:OE2	2.07	0.55
1:F:201:PHE:CE2	1:F:205:ILE:HD11	2.41	0.54
1:J:70:THR:OG1	1:J:79:ILE:CG1	2.51	0.54
1:B:-2:MET:O	1:B:0:SER:N	2.40	0.54
1:E:27:MET:HE1	1:E:30:VAL:HG21	1.90	0.54
1:I:49:TYR:CD1	1:I:100:VAL:HG11	2.43	0.54
1:J:182:PHE:HE1	1:J:186:ILE:HG22	1.21	0.54
1:J:70:THR:HB	1:J:79:ILE:CG1	2.38	0.54
1:E:213:GLU:CD	1:E:213:GLU:H	2.11	0.53
1:J:222:ILE:O	1:J:225:LEU:HB2	2.09	0.53
1:I:38:SER:N	1:I:41:GLU:OE1	2.33	0.53
1:F:166:GLN:NE2	1:F:210:THR:CG2	2.72	0.52
1:I:6:GLN:O	1:I:9:GLN:N	2.41	0.52
1:J:216:TYR:HD1	1:J:217:LYS:HB2	1.72	0.52
1:I:67:GLU:OE1	1:I:86:ARG:HD3	2.10	0.52
1:I:81:MET:HE1	1:J:6:GLN:CG	2.39	0.52
1:J:69:LYS:HE2	1:J:73:ASP:OD2	2.08	0.52
1:A:42:ARG:HD3	3:A:310:HOH:O	2.09	0.52
1:F:201:PHE:CE2	1:F:205:ILE:CD1	2.92	0.52
1:J:226:LEU:HA	1:J:229:ASN:HB2	1.91	0.52
1:J:3:ASP:OD2	1:J:5:GLU:HG2	2.10	0.52
1:A:4:ARG:NH2	1:A:41:GLU:OE1	2.40	0.52
1:E:82:VAL:HG22	1:F:13:LEU:HD11	1.92	0.52
1:J:70:THR:CB	1:J:79:ILE:CG1	2.89	0.51
1:I:4:ARG:O	1:I:5:GLU:C	2.47	0.51
1:I:234:THR:O	1:I:236:ASP:N	2.40	0.51
1:I:2:VAL:HG12	1:I:3:ASP:H	1.74	0.51
1:J:216:TYR:CD1	1:J:217:LYS:CB	2.94	0.51
1:I:49:TYR:CZ	1:I:100:VAL:HG12	2.46	0.50
1:B:163:GLU:HB3	1:B:164:HIS:CD2	2.47	0.50
1:F:4:ARG:NH2	1:F:41:GLU:OE1	2.44	0.50
1:J:113:SER:HB3	1:J:115:THR:HG22	1.92	0.50
1:J:163:GLU:HG3	1:J:164:HIS:CD2	2.46	0.50
1:F:60:TRP:CE2	1:F:137:VAL:HG12	2.47	0.50
1:B:207:GLU:O	1:B:209:ASP:N	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:SER:N	1:E:116:GLN:OE1	2.34	0.50
1:J:183:TYR:HE2	1:J:196:LEU:HD21	1.76	0.50
1:B:143:ARG:O	1:B:146:VAL:CG2	2.59	0.50
1:B:60:TRP:CE2	1:B:137:VAL:HG12	2.47	0.50
1:E:205:ILE:HA	1:E:208:LEU:HD13	1.94	0.49
1:F:3:ASP:HB3	1:F:6:GLN:HB2	1.93	0.49
1:E:83:ARG:NH1	1:E:87:GLU:OE2	2.45	0.49
1:J:60:TRP:CD1	1:J:90:GLU:HG3	2.47	0.49
1:I:66:ILE:O	1:I:70:THR:HG23	2.13	0.49
1:J:216:TYR:CD1	1:J:216:TYR:C	2.85	0.49
1:F:212:ASN:O	1:F:214:ASP:N	2.46	0.49
1:J:115:THR:HG23	1:J:116:GLN:H	1.75	0.49
1:I:81:MET:CE	1:J:6:GLN:HG2	2.40	0.49
1:J:182:PHE:O	1:J:187:GLN:N	2.39	0.49
1:J:161:SER:HB2	1:J:172:ARG:HG3	1.94	0.48
1:J:222:ILE:O	1:J:226:LEU:HG	2.13	0.48
1:I:179:TYR:O	1:I:182:PHE:HB3	2.14	0.48
1:E:105:ASP:OD1	1:E:127:LYS:NZ	2.44	0.48
1:B:231:THR:O	1:B:234:THR:CG2	2.32	0.48
1:I:15:GLU:HB2	1:I:23:MET:SD	2.54	0.48
1:I:81:MET:CE	1:J:6:GLN:CG	2.91	0.48
1:A:212:ASN:HD21	1:A:214:ASP:HB2	1.79	0.48
1:B:69:LYS:N	1:B:69:LYS:HD3	2.28	0.48
1:F:50:LYS:NZ	2:G:798:PRO:HG3	2.28	0.48
1:J:104:LEU:HA	1:J:108:LEU:HB2	1.95	0.48
1:J:220:THR:O	1:J:223:MET:CB	2.58	0.48
1:A:178:ASN:OD1	2:C:768:SEP:HB3	2.14	0.48
1:F:26:ALA:O	1:F:30:VAL:HG23	2.14	0.48
1:I:78:LYS:O	1:I:82:VAL:HG23	2.15	0.47
1:J:104:LEU:HD13	1:J:127:LYS:HG2	1.95	0.47
1:E:178:ASN:OD1	2:G:769:VAL:HG23	2.14	0.47
1:A:122:PHE:HE1	1:A:126:MET:HE1	1.79	0.47
1:A:4:ARG:HH21	1:A:41:GLU:CD	2.17	0.47
1:J:182:PHE:HD1	1:J:186:ILE:HG13	1.80	0.47
1:B:132:ARG:O	1:B:136:GLU:HG3	2.15	0.47
1:I:104:LEU:HD23	1:I:108:LEU:HD12	1.96	0.47
1:B:-2:MET:HA	1:B:1:MET:HE2	1.93	0.46
1:F:212:ASN:O	1:F:213:GLU:C	2.52	0.46
1:I:43:ASN:O	1:I:47:VAL:HG23	2.16	0.46
1:I:49:TYR:CE1	1:I:100:VAL:HG12	2.50	0.46
1:J:113:SER:CB	1:J:115:THR:HG22	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:125:LYS:HD2	1:J:175:LEU:HA	1.98	0.46
1:A:66:ILE:O	1:A:70:THR:HG23	2.16	0.46
1:E:208:LEU:HD12	1:E:208:LEU:HA	1.83	0.46
1:B:230:LEU:HA	1:B:230:LEU:HD23	1.76	0.46
1:F:50:LYS:HG2	2:G:798:PRO:HB3	1.98	0.46
1:B:110:LYS:HB2	1:B:110:LYS:HE3	1.72	0.45
1:I:22:ASP:O	1:I:25:ALA:HB3	2.17	0.45
1:B:201:PHE:HE1	1:B:223:MET:HB3	1.82	0.45
1:E:143:ARG:O	1:E:147:VAL:HG23	2.16	0.45
1:E:3:ASP:OD1	1:E:4:ARG:N	2.49	0.45
1:E:78:LYS:O	1:E:81:MET:HB3	2.16	0.45
1:E:101:LEU:HD13	1:E:131:TYR:CZ	2.51	0.45
1:I:2:VAL:CG1	1:I:3:ASP:N	2.70	0.45
1:I:19:ARG:O	1:I:22:ASP:HB2	2.16	0.45
1:J:177:LEU:HD22	1:J:222:ILE:HG23	1.98	0.45
1:J:195:HIS:O	1:J:199:THR:HG23	2.17	0.45
1:F:166:GLN:OE1	1:F:210:THR:HG21	2.17	0.45
1:J:115:THR:CG2	1:J:116:GLN:N	2.80	0.44
1:J:170:PRO:O	1:J:171:ILE:C	2.55	0.44
1:J:201:PHE:O	1:J:201:PHE:CD1	2.70	0.44
1:B:113:SER:OG	1:B:115:THR:HG23	2.17	0.44
1:F:166:GLN:CD	1:F:210:THR:CG2	2.85	0.44
1:B:117:TYR:O	1:B:121:VAL:HG23	2.18	0.44
1:I:23:MET:HG2	1:I:48:ALA:HB2	1.99	0.44
1:B:143:ARG:O	1:B:147:VAL:HG23	2.18	0.44
1:F:75:ASN:C	1:F:79:ILE:HD12	2.38	0.44
1:I:37:LEU:HD13	1:I:108:LEU:HD21	1.99	0.44
1:J:23:MET:HG2	1:J:48:ALA:HB2	1.99	0.44
1:J:79:ILE:O	1:J:79:ILE:HG22	2.17	0.44
1:I:39:ASN:N	1:I:39:ASN:OD1	2.47	0.44
1:B:13:LEU:HA	1:B:13:LEU:HD12	1.78	0.43
1:I:77:LYS:NZ	1:I:80:GLU:OE2	2.39	0.43
1:J:172:ARG:NH2	1:J:203:ASP:OD2	2.51	0.43
1:J:201:PHE:CD1	1:J:223:MET:SD	3.11	0.43
1:J:197:ALA:HB3	1:J:230:LEU:HD21	1.99	0.43
1:I:28:LYS:O	1:I:32:GLU:CG	2.66	0.43
1:J:182:PHE:O	1:J:186:ILE:CB	2.59	0.43
1:E:57:ARG:NH2	1:E:136:GLU:OE2	2.47	0.43
1:F:129:ASP:OD1	1:F:178:ASN:ND2	2.47	0.43
1:F:143:ARG:O	1:F:147:VAL:HG23	2.18	0.43
1:J:183:TYR:CE2	1:J:196:LEU:HD21	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:127:LYS:HD3	1:I:153:ALA:HB2	2.00	0.43
1:I:77:LYS:HA	1:I:77:LYS:HD2	1.74	0.43
1:J:189:ALA:HB1	1:J:192:GLN:HG3	2.00	0.43
1:E:177:LEU:HD23	2:G:769:VAL:HG22	2.00	0.43
1:E:60:TRP:NE1	1:E:90:GLU:HG3	2.34	0.43
1:F:166:GLN:NE2	1:F:210:THR:HG22	2.34	0.43
1:I:6:GLN:HA	1:I:9:GLN:HG2	1.99	0.43
1:A:90:GLU:O	1:A:94:GLU:HG3	2.18	0.43
1:B:-2:MET:C	1:B:0:SER:N	2.72	0.43
1:J:98:GLN:HG3	1:J:99:ASP:N	2.33	0.43
1:F:2:VAL:HG12	1:F:3:ASP:N	2.33	0.43
1:B:103:LEU:HD23	1:B:103:LEU:HA	1.77	0.43
2:C:796:LEU:HG	2:C:797:ALA:N	2.34	0.43
1:E:8:VAL:HA	1:E:27:MET:HE3	2.01	0.43
1:F:230:LEU:O	1:F:234:THR:HG23	2.18	0.43
1:B:156:GLU:O	1:B:160:ILE:HG13	2.19	0.43
1:B:230:LEU:O	1:B:234:THR:HB	2.19	0.43
1:B:78:LYS:O	1:B:81:MET:HB3	2.19	0.43
1:I:33:LEU:O	1:I:34:ASN:HB3	2.19	0.42
1:J:86:ARG:NH1	1:J:86:ARG:HB3	2.34	0.42
1:B:167:PRO:HA	1:B:172:ARG:HD3	2.01	0.42
1:B:163:GLU:OE1	1:B:164:HIS:NE2	2.53	0.42
1:E:42:ARG:HD2	1:E:122:PHE:CD2	2.54	0.42
1:I:2:VAL:HG13	1:I:3:ASP:OD1	2.16	0.42
1:I:75:ASN:O	1:I:79:ILE:HG13	2.19	0.42
1:J:175:LEU:O	1:J:179:TYR:HB2	2.19	0.42
1:J:174:GLY:HA2	1:J:177:LEU:HB3	2.01	0.42
1:J:76:GLU:OE2	1:J:79:ILE:CD1	2.67	0.42
1:B:86:ARG:HG2	1:B:86:ARG:HH11	1.85	0.42
1:E:209:ASP:OD1	1:E:210:THR:N	2.52	0.42
1:A:118:GLU:HG2	1:A:165:MET:CE	2.49	0.42
1:B:161:SER:HB2	1:B:172:ARG:HG3	2.02	0.42
1:F:161:SER:O	1:F:165:MET:HB2	2.20	0.42
1:I:3:ASP:O	1:I:6:GLN:HB2	2.19	0.42
1:E:127:LYS:HG2	1:E:153:ALA:CB	2.49	0.42
1:E:231:THR:O	1:E:234:THR:CG2	2.67	0.42
1:F:166:GLN:HE22	1:F:210:THR:HG22	1.83	0.42
1:J:50:LYS:NZ	2:K:795:SEP:O1P	2.53	0.42
1:A:168:THR:HB	1:A:211:LEU:HD23	2.01	0.42
1:E:220:THR:O	1:E:224:GLN:HG3	2.19	0.42
1:J:108:LEU:HD22	1:J:123:TYR:CZ	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:234:THR:C	1:I:236:ASP:N	2.73	0.41
1:A:63:ILE:HD11	1:B:17:ALA:HB2	2.01	0.41
1:B:62:VAL:O	1:B:66:ILE:HG13	2.19	0.41
1:J:226:LEU:H	1:J:226:LEU:HG	1.70	0.41
1:B:-2:MET:C	1:B:0:SER:H	2.24	0.41
1:E:132:ARG:HG3	1:E:186:ILE:HG13	2.02	0.41
1:E:63:ILE:HD12	1:F:13:LEU:HD22	2.02	0.41
1:F:166:GLN:OE1	1:F:210:THR:CG2	2.68	0.41
1:J:70:THR:HB	1:J:79:ILE:HG12	1.99	0.41
1:J:196:LEU:HA	1:J:199:THR:OG1	2.20	0.41
1:J:224:GLN:O	1:J:227:ARG:HB3	2.19	0.41
1:J:60:TRP:CE2	1:J:137:VAL:HG12	2.56	0.41
1:J:170:PRO:O	1:J:173:LEU:N	2.53	0.41
1:B:4:ARG:HH21	1:B:41:GLU:CD	2.24	0.41
1:I:29:ASN:CA	1:I:32:GLU:HG3	2.47	0.41
1:B:96:VAL:O	1:B:100:VAL:HG23	2.21	0.41
1:I:28:LYS:O	1:I:32:GLU:HG2	2.20	0.41
1:E:234:THR:HG23	1:E:235:SER:N	2.36	0.41
1:J:70:THR:HB	1:J:79:ILE:HG13	2.02	0.41
1:B:124:LEU:HA	1:B:124:LEU:HD23	1.93	0.40
1:J:166:GLN:HA	1:J:167:PRO:HD3	1.88	0.40
1:A:61:ARG:NH1	3:A:304:HOH:O	2.51	0.40
1:E:212:ASN:O	1:E:216:TYR:HB3	2.22	0.40
1:B:129:ASP:O	1:B:132:ARG:HB3	2.21	0.40
1:J:83:ARG:HA	1:J:86:ARG:NH1	2.32	0.40
1:I:125:LYS:HD2	1:I:175:LEU:HA	2.04	0.40
1:I:33:LEU:O	1:I:34:ASN:CB	2.70	0.40
1:I:3:ASP:HB2	1:I:6:GLN:HG2	2.04	0.40
1:J:183:TYR:HB3	1:J:193:ALA:HB2	2.02	0.40
1:J:201:PHE:HD1	1:J:223:MET:SD	2.44	0.40
1:J:92:GLU:O	1:J:96:VAL:HG23	2.21	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:224:GLN:CD	1:J:224:GLN:OE1[8_665]	0.42	1.78
1:J:224:GLN:OE1	1:J:224:GLN:NE2[8_665]	0.92	1.28
1:J:224:GLN:CD	1:J:224:GLN:CD[8_665]	0.99	1.21
1:J:224:GLN:OE1	1:J:224:GLN:OE1[8_665]	1.55	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:224:GLN:CG	1:J:224:GLN:OE1[8_665]	1.68	0.52
1:J:224:GLN:CD	1:J:224:GLN:NE2[8_665]	1.85	0.35
1:B:76:GLU:OE1	1:I:39:ASN:OD1[5_545]	1.92	0.28
1:B:76:GLU:CD	1:I:39:ASN:OD1[5_545]	1.95	0.25
1:F:118:GLU:OE2	1:I:71:SER:OG[1_455]	2.07	0.13

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	234/241 (97%)	229 (98%)	5 (2%)	0	100 100
1	B	236/241 (98%)	229 (97%)	6 (2%)	1 (0%)	39 72
1	E	234/241 (97%)	231 (99%)	3 (1%)	0	100 100
1	F	237/241 (98%)	233 (98%)	4 (2%)	0	100 100
1	I	233/241 (97%)	228 (98%)	5 (2%)	0	100 100
1	J	220/241 (91%)	207 (94%)	13 (6%)	0	100 100
2	C	5/40 (12%)	4 (80%)	0	1 (20%)	0 0
2	G	5/40 (12%)	4 (80%)	1 (20%)	0	100 100
2	K	1/40 (2%)	1 (100%)	0	0	100 100
All	All	1405/1566 (90%)	1366 (97%)	37 (3%)	2 (0%)	56 86

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	767	GLN
1	B	-1	GLY

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	208/212 (98%)	206 (99%)	2 (1%)	82 95
1	B	209/212 (99%)	206 (99%)	3 (1%)	74 92
1	E	208/212 (98%)	207 (100%)	1 (0%)	92 97
1	F	210/212 (99%)	208 (99%)	2 (1%)	82 95
1	I	207/212 (98%)	206 (100%)	1 (0%)	92 97
1	J	196/212 (92%)	195 (100%)	1 (0%)	92 97
2	C	8/33 (24%)	8 (100%)	0	100 100
2	G	8/33 (24%)	8 (100%)	0	100 100
2	K	3/33 (9%)	3 (100%)	0	100 100
All	All	1257/1371 (92%)	1247 (99%)	10 (1%)	86 96

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	SER
1	A	179	TYR
1	B	1	MET
1	B	70	THR
1	B	179	TYR
1	E	179	TYR
1	F	179	TYR
1	F	221	LEU
1	I	39	ASN
1	J	179	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	6	GLN
1	F	9	GLN
1	F	116	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	6	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	$\#\|Z\| > 2$
2	SEP	C	768	2	7,9,10	1.67	1 (14%)	8,12,14	1.53	2 (25%)
2	SEP	C	795	2	7,9,10	2.07	3 (42%)	8,12,14	2.04	3 (37%)
2	SEP	G	768	2	7,9,10	2.10	4 (57%)	8,12,14	2.45	4 (50%)
2	SEP	G	795	2	7,9,10	2.28	4 (57%)	8,12,14	1.48	0
2	SEP	K	768	2	7,9,10	1.63	1 (14%)	8,12,14	1.42	1 (12%)
2	SEP	K	795	-	7,9,10	1.78	2 (28%)	8,12,14	1.67	1 (12%)

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	SEP	C	768	2	-	0/5/8/10	0/0/0/0
2	SEP	C	795	2	-	0/5/8/10	0/0/0/0
2	SEP	G	768	2	-	0/5/8/10	0/0/0/0
2	SEP	G	795	2	-	0/5/8/10	0/0/0/0
2	SEP	K	768	2	-	0/5/8/10	0/0/0/0
2	SEP	K	795	-	-	0/5/8/10	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	768	SEP	P-O2P	-3.35	1.43	1.54
2	G	795	SEP	P-O3P	-3.35	1.43	1.54
2	C	795	SEP	P-O2P	-3.21	1.43	1.54
2	G	795	SEP	P-O2P	-3.10	1.44	1.54
2	C	795	SEP	P-O3P	-3.03	1.44	1.54
2	G	768	SEP	P-O3P	-2.93	1.44	1.54
2	G	795	SEP	P-O1P	-2.76	1.42	1.50
2	G	795	SEP	P-OG	-2.40	1.53	1.59
2	G	768	SEP	P-O1P	-2.25	1.43	1.50
2	C	795	SEP	P-O1P	-2.19	1.43	1.50
2	G	768	SEP	P-OG	-2.18	1.53	1.59
2	K	795	SEP	P-O2P	2.17	1.62	1.54
2	K	768	SEP	P-O1P	3.29	1.61	1.50
2	C	768	SEP	P-O1P	3.33	1.61	1.50
2	K	795	SEP	P-O1P	3.40	1.61	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	768	SEP	OG-P-O1P	-3.18	99.08	107.08
2	G	768	SEP	O-C-CA	-2.43	119.19	125.72
2	K	768	SEP	O-C-CA	-2.42	119.22	125.72
2	C	768	SEP	O-C-CA	-2.21	119.79	125.72
2	C	795	SEP	O-C-CA	-2.05	120.21	125.72
2	G	768	SEP	O2P-P-O1P	2.21	117.83	110.63
2	C	795	SEP	O3P-P-O2P	2.26	115.75	107.44
2	C	768	SEP	O3P-P-OG	2.43	113.82	106.72
2	C	795	SEP	OG-CB-CA	3.41	111.23	108.26
2	K	795	SEP	OG-CB-CA	4.04	111.78	108.26
2	G	768	SEP	OG-CB-CA	4.56	112.23	108.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	768	SEP	1	0
2	K	795	SEP	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	235/241 (97%)	-0.24	5 (2%) 67 61	25, 43, 85, 126	0
1	B	238/241 (98%)	-0.04	9 (3%) 44 37	30, 56, 106, 139	0
1	E	234/241 (97%)	-0.25	4 (1%) 73 68	24, 48, 85, 119	0
1	F	238/241 (98%)	-0.16	1 (0%) 93 92	24, 46, 87, 106	0
1	I	235/241 (97%)	-0.19	4 (1%) 73 68	25, 58, 96, 126	0
1	J	224/241 (92%)	0.94	47 (20%) 1 1	47, 104, 146, 162	0
2	C	9/40 (22%)	1.11	3 (33%) 0 0	62, 75, 96, 100	0
2	G	9/40 (22%)	0.54	0 100 100	46, 69, 105, 105	0
2	K	3/40 (7%)	0.48	0 100 100	57, 57, 72, 84	0
All	All	1425/1566 (90%)	0.02	73 (5%) 32 24	24, 55, 124, 162	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	230	LEU	5.7
1	J	203	ASP	5.7
1	B	211	LEU	5.7
1	J	232	LEU	4.7
2	C	793	LYS	4.7
1	J	117	TYR	4.5
1	J	202	ASP	4.3
1	J	139	THR	4.2
1	A	73	ASP	3.9
1	J	78	LYS	3.8
1	J	194	CYS	3.7
1	J	191	GLU	3.7
1	J	71	SER	3.7
1	A	70	THR	3.7
1	J	233	TRP	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	113	SER	3.4
1	E	73	ASP	3.1
1	B	213	GLU	3.1
1	J	192	GLN	3.0
2	C	798	PRO	3.0
1	J	204	ALA	3.0
1	B	214	ASP	2.9
1	J	62	VAL	2.9
1	B	212	ASN	2.9
1	I	236	ASP	2.9
1	E	72	ALA	2.9
1	J	115	THR	2.9
1	J	66	ILE	2.9
1	B	210	THR	2.8
1	J	231	THR	2.8
1	J	140	GLY	2.8
1	J	116	GLN	2.8
1	J	168	THR	2.8
1	J	201	PHE	2.8
1	J	73	ASP	2.8
2	C	766	ARG	2.8
1	J	227	ARG	2.7
1	J	144	ALA	2.7
1	I	13	LEU	2.7
1	J	164	HIS	2.6
1	J	141	GLU	2.6
1	J	74	GLY	2.6
1	J	167	PRO	2.6
1	B	216	TYR	2.6
1	J	64	SER	2.5
1	E	69	LYS	2.5
1	J	68	GLN	2.5
1	J	163	GLU	2.4
1	J	234	THR	2.4
1	J	138	ALA	2.4
1	A	74	GLY	2.3
1	J	124	LEU	2.3
1	B	205	ILE	2.3
1	I	235	SER	2.3
1	J	183	TYR	2.3
1	J	147	VAL	2.2
1	J	69	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	209	ASP	2.2
1	J	185	GLU	2.2
1	J	184	TYR	2.1
1	A	72	ALA	2.1
1	J	188	ASN	2.1
1	E	71	SER	2.1
1	J	228	ASP	2.1
1	J	207	GLU	2.1
1	I	6	GLN	2.1
1	J	220	THR	2.1
1	J	229	ASN	2.1
1	F	70	THR	2.1
1	B	194	CYS	2.0
1	J	226	LEU	2.0
1	J	70	THR	2.0
1	A	76	GLU	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
2	SEP	K	795	10/11	0.92	0.17	-	86,104,117,117	0
2	SEP	C	795	10/11	0.98	0.12	-	39,55,66,69	0
2	SEP	G	768	10/11	0.97	0.15	-	39,47,63,70	0
2	SEP	C	768	10/11	0.97	0.15	-	40,52,55,61	0
2	SEP	G	795	10/11	0.98	0.13	-	33,43,47,57	0
2	SEP	K	768	10/11	0.97	0.13	-	36,48,61,62	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.