W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:20 PM GMT

PDB ID	:	1F3U
Title	:	CRYSTAL STRUCTURE OF THE RAP30/74 INTERACTION DOMAINS OF HUMAN TFIIF
Authors	:	Gaiser, F.; Tan, S.; Richmond, T.J.
Deposited on	:	2000-06-06
Resolution	:	1.70 Å(reported)

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

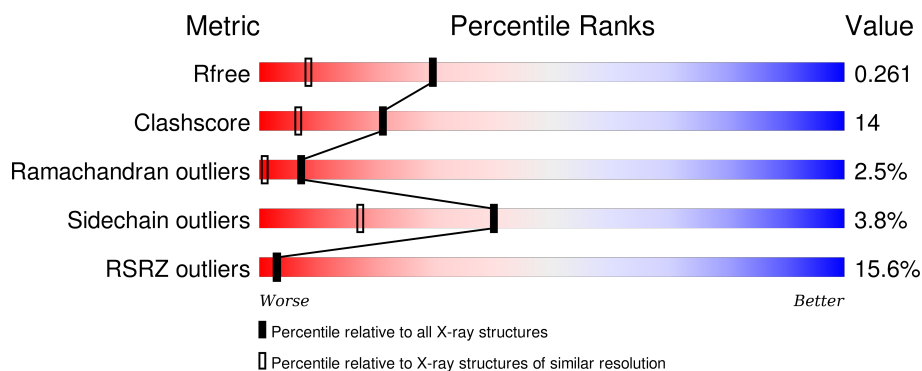|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 1.70 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	Percentile Ranks	Value
Rfree		0.261
Clashscore		14
Ramachandran outliers		2.5%
Sidechain outliers		3.8%
RSRZ outliers		15.6%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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	118	8% / 79% / 19% / •
1	C	118	24% / 65% / 31% / •
1	E	118	6% / 78% / 19% / •
1	G	118	14% / 82% / 17% / •
2	B	171	9% / 61% / 19% / • / 19%

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Mol	Chain	Length	Quality of chain
2	D	171	16% / 63% / 25% / 11%
2	F	171	14% / 68% / 20% / 10%
2	H	171	19% / 57% / 20% / 20%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9192 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 TRANSCRIPTION INITIATION FACTOR IIF, BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	118	Total 895	C 557	N 163	O 174	S 1	16	0	0
1	C	118	Total 894	C 557	N 163	O 173	S 1	21	0	0
1	E	118	Total 895	C 557	N 163	O 174	S 1	0	0	0
1	G	118	Total 895	C 557	N 163	O 174	S 1	5	0	0

- Molecule 2 is a protein called TRANSCRIPTION INITIATION FACTOR IIF, ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	139	Total 1158	C 737	N 213	O 205	S 3	22	0	0
2	D	153	Total 1284	C 812	N 235	O 234	S 3	14	0	0
2	F	154	Total 1310	C 827	N 240	O 240	S 3	90	8	0
2	H	137	Total 1169	C 743	N 215	O 208	S 3	52	6	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	95	Total 95	O 95	0	0
3	B	89	Total 89	O 89	0	0
3	C	52	Total 52	O 52	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	91	Total 91	O 91	0	0
3	E	118	Total 118	O 118	0	0
3	F	119	Total 119	O 119	0	0
3	G	71	Total 71	O 71	0	0
3	H	57	Total 57	O 57	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: TRANSCRIPTION INITIATION FACTOR IIF, BETA SUBUNIT
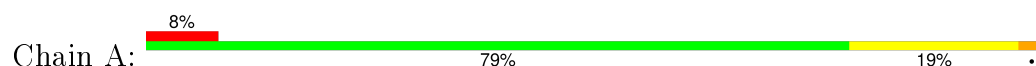
- Molecule 1: TRANSCRIPTION INITIATION FACTOR IIF, BETA SUBUNIT
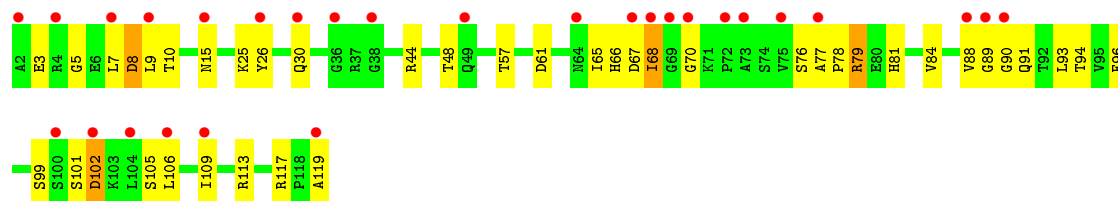
- Molecule 1: TRANSCRIPTION INITIATION FACTOR IIF, BETA SUBUNIT
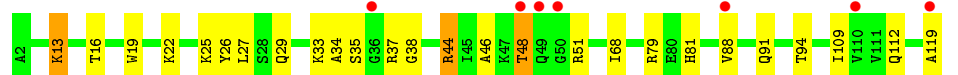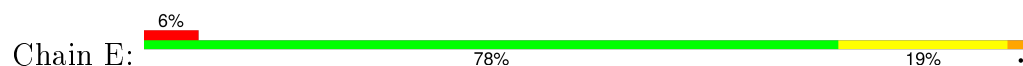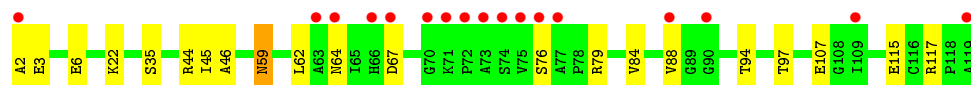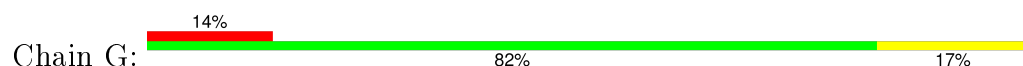

- Molecule 1: TRANSCRIPTION INITIATION FACTOR IIF, BETA SUBUNIT

- Molecule 2: TRANSCRIPTION INITIATION FACTOR IIF, ALPHA SUBUNIT

P93 E94 D95 Q96 R101 K105 K109 T119 E120 I126 F127 T128 N142 L149 R153 THR LEU THR ALA GLU GLU ALA GLU GLU TRP GLU ARG ARG ASN LYS VAL LEU ASN

● Molecule 2: TRANSCRIPTION INITIATION FACTOR IIF, ALPHA SUBUNIT

Chain D:

ALA ALA LEU GLY PRO S7 S8 Q9 E13 P19 K20 N21 T22 T23 M29 A30 F31 A34 D35 K36 V37 N38 F39 A40 T41 Q44 A45 R46 L47 N53 K54 K55 I56 P63 GLU SER GLY ALA GLY SER GLU PHE ASN R73 K74 E77 E78 A79 K82 K89

E90 F91 R92 E94 D95 Q96 P97 W98 L99 G104 K105 S106 G107 R108 G116 N121 T122 S123 P131 T154 L155 T156 A157 E158 E159 A160 E161 E162 E163 W164 E165 R166 R167 N168 LYS VAL LEU ASN

● Molecule 2: TRANSCRIPTION INITIATION FACTOR IIF, ALPHA SUBUNIT

Chain F:

ALA ALA LEU G5 P6 S7 S8 Q9 N10 V11 T12 E13 K20 N21 F31 V37 N38 F39 A40 T41 L51 K54 K55 M62 PRO GLU SER GLY ALA GLY SER GLU PHE ASN R73 K74 L75 R76 E77 E78 A79 R80 R81 K82 K89 E90 F91 E94 D95 Q96 L99

V102 G107 G117 V118 D132 R153 T154 L155 E159 A160 E161 E162 E163 W164 E165 R166 R167 N168 LYS VAL LEU ASN

● Molecule 2: TRANSCRIPTION INITIATION FACTOR IIF, ALPHA SUBUNIT

Chain H:

ALA ALA LEU GLY PRO S7 S8 Q9 N10 V11 T12 K25 Y26 N27 N38 F39 W42 N43 Q44 D50 L51 S52 N53 K54 K55 I56 Y57 Q58 E59 E60 E61 M62 PRO GLU SER GLY ALA GLY SER GLU PHE ASN R73 K74 E77 E78 A79 R80 R81 K82 K83 Y84 G85 I86 V87

L88 K89 E90 F91 R92 P93 E94 D95 Q96 P97 W98 L99 L100 R101 V102 N103 G104 G107 K111 K114 E120 N121 T122 F135 H141 N142 T147 H152 R153 THR LEU THR ALA GLU GLU ALA GLU GLU TRP GLU ARG ARG ASN LYS VAL LEU ASN

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	48.02Å 72.29Å 82.27Å 104.51° 93.32° 104.32°	Depositor
Resolution (Å)	6.00 – 1.70 67.37 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.4 (6.00-1.70) 87.8 (67.37-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 1.70Å)	Xtriage
Refinement program	CNS 0.9A	Depositor
R, R_{free}	0.225 , 0.260 0.228 , 0.261	Depositor DCC
R_{free} test set	4273 reflections (4.02%)	DCC
Wilson B-factor (Å^2)	29.7	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 71.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 108913 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9192	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.23 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.1801e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 (i)

5.1 Standard geometry (i)

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	0.33	0/909	0.65	0/1227
1	C	0.30	0/908	0.67	0/1226
1	E	0.38	0/909	0.71	1/1227 (0.1%)
1	G	0.33	0/909	0.63	0/1227
2	B	0.35	0/1186	0.68	0/1594
2	D	0.31	0/1314	0.60	0/1768
2	F	0.38	0/1340	0.65	0/1804
2	H	0.34	0/1196	0.61	0/1608
All	All	0.34	0/8671	0.65	1/11681 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	38	GLY	N-CA-C	5.22	126.16	113.10

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	895	0	904	25	0
1	C	894	0	901	33	0
1	E	895	0	904	29	0
1	G	895	0	904	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1158	0	1151	35	0
2	D	1284	0	1261	42	0
2	F	1310	0	1283	34	0
2	H	1169	0	1162	47	0
3	A	95	0	0	1	0
3	B	89	0	0	7	0
3	C	52	0	0	2	0
3	D	91	0	0	2	0
3	E	118	0	0	4	0
3	F	119	0	0	2	0
3	G	71	0	0	2	0
3	H	57	0	0	1	0
All	All	9192	0	8470	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 14.

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)
2:D:56:ILE:HD11	2:D:161:GLU:HG2	1.52	0.88
1:A:59:ASN:HD21	1:A:62:LEU:HD13	1.40	0.86
2:B:51:LEU:HD22	2:B:91:PHE:HZ	1.43	0.83
2:D:21:ASN:HD22	2:D:21:ASN:C	1.84	0.80
1:G:59:ASN:HD22	1:G:59:ASN:C	1.87	0.78
1:A:84:VAL:HG21	1:A:117:ARG:HE	1.51	0.76
2:H:10[A]:ASN:O	2:H:11[A]:VAL:HB	1.85	0.75
2:D:54:LYS:HD3	2:D:55:LYS:HD3	1.68	0.74
2:D:162:GLU:O	2:D:166:ARG:HG2	1.88	0.73
2:F:54:LYS:HG2	3:F:236:HOH:O	1.86	0.73
1:G:59:ASN:ND2	1:G:62:LEU:H	1.87	0.73
2:F:96:GLN:HE21	2:F:96:GLN:HA	1.53	0.72
1:A:88:VAL:HG23	3:A:161:HOH:O	1.90	0.72
2:D:54:LYS:HG2	3:D:276:HOH:O	1.90	0.72
1:E:46:ALA:HB2	2:F:11[A]:VAL:HG22	1.72	0.72
1:G:44:ARG:HG3	2:H:11[B]:VAL:HG11	1.73	0.70
1:E:94:THR:HG21	2:F:39:PHE:CZ	2.26	0.70
1:G:76:SER:HB2	1:G:79:ARG:HH21	1.57	0.69
1:G:59:ASN:HD21	1:G:62:LEU:H	1.38	0.69
1:C:101:SER:O	1:C:102:ASP:HB2	1.90	0.69
1:C:88:VAL:HB	1:C:113:ARG:HG3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:22:LYS:NZ	2:H:122:THR:HG21	2.08	0.69
2:B:21:ASN:HB3	2:F:132:ASP:HA	1.74	0.68
2:D:56:ILE:HG23	2:D:89:LYS:HB2	1.75	0.68
1:G:22:LYS:HE3	1:G:115:GLU:HG3	1.75	0.68
1:A:94:THR:HG21	2:B:39:PHE:CZ	2.31	0.66
1:E:34:ALA:O	2:F:20:LYS:HD2	1.95	0.66
1:G:84:VAL:HG21	1:G:117:ARG:NH1	2.10	0.66
2:F:73:ARG:HG2	2:F:74:LYS:H	1.61	0.66
2:B:90:GLU:H	2:B:90:GLU:CD	2.00	0.66
2:B:54:LYS:HD3	2:B:91:PHE:CD1	2.33	0.63
1:C:5:GLY:O	2:D:46:ARG:HA	1.98	0.63
1:C:66:HIS:HB3	1:C:70:GLY:HA3	1.79	0.63
2:H:74:LYS:HD2	2:H:74:LYS:H	1.63	0.63
1:A:22:LYS:HD3	1:A:115:GLU:HG3	1.80	0.63
1:E:44:ARG:HG2	2:F:13:GLU:HG2	1.81	0.63
2:H:102:VAL:O	2:H:107:GLY:HA3	1.98	0.63
1:G:97:THR:HG23	1:G:107:GLU:HG3	1.79	0.63
2:B:101:ARG:HD2	3:B:201:HOH:O	1.99	0.62
2:H:56:ILE:HG12	2:H:57:TYR:N	2.15	0.62
1:C:94:THR:HG21	2:D:39:PHE:CZ	2.34	0.62
2:D:21:ASN:O	2:D:21:ASN:ND2	2.27	0.62
1:A:37:ARG:HH11	1:A:37:ARG:HG3	1.65	0.62
1:C:105:SER:HB2	3:C:133:HOH:O	2.00	0.61
2:H:50:ASP:O	2:H:96:GLN:HG3	2.00	0.61
1:G:44:ARG:HG2	2:H:11[A]:VAL:HG21	1.82	0.61
2:H:10[B]:ASN:O	2:H:11[B]:VAL:HG23	2.02	0.60
2:B:21:ASN:HB3	2:F:132:ASP:CB	2.31	0.60
1:G:76:SER:CB	1:G:79:ARG:HH21	2.15	0.60
2:B:51:LEU:HD22	2:B:91:PHE:CZ	2.32	0.59
1:G:44:ARG:NH1	2:H:11[B]:VAL:HG21	2.17	0.59
2:H:74:LYS:HD2	2:H:74:LYS:N	2.17	0.59
1:G:22:LYS:HZ2	2:H:122:THR:HG21	1.66	0.59
2:D:31:PHE:CD2	2:D:37:VAL:HG21	2.38	0.59
2:H:111:LYS:HD3	2:H:152:HIS:CD2	2.36	0.59
1:E:94:THR:HG22	1:E:109:ILE:HD12	1.84	0.59
2:D:157:ALA:O	2:D:161:GLU:HG3	2.03	0.58
1:C:88:VAL:HG22	1:C:88:VAL:O	2.03	0.58
1:E:88:VAL:HG23	3:E:409:HOH:O	2.03	0.58
1:E:22:LYS:NZ	3:E:536:HOH:O	2.37	0.58
1:C:84:VAL:HG21	1:C:117:ARG:HE	1.66	0.58
1:C:93:LEU:O	1:C:109:ILE:HD12	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:44:ARG:HH11	2:H:11[B]:VAL:HG21	1.69	0.58
2:H:11[B]:VAL:CG1	2:H:12[B]:THR:N	2.67	0.57
2:F:163:GLU:O	2:F:167:ARG:HG2	2.05	0.57
1:E:79:ARG:CZ	1:E:119:ALA:O	2.53	0.57
2:H:25:LYS:HE3	3:H:664:HOH:O	2.04	0.57
2:H:54:LYS:C	2:H:56:ILE:H	2.08	0.57
1:A:101:SER:O	1:A:102:ASP:HB2	2.05	0.57
2:H:11[B]:VAL:HG12	2:H:12[B]:THR:N	2.21	0.56
2:H:92:ARG:HD3	2:H:92:ARG:H	1.68	0.56
2:H:92:ARG:HD3	2:H:92:ARG:N	2.20	0.56
2:B:6:PRO:HA	3:B:243:HOH:O	2.05	0.56
2:B:21:ASN:HB3	2:F:132:ASP:CA	2.35	0.56
2:D:36:LYS:HB2	2:D:36:LYS:NZ	2.21	0.56
2:B:61:GLU:OE2	2:B:82:LYS:HD3	2.06	0.56
2:H:56:ILE:CG1	2:H:57:TYR:N	2.70	0.55
2:H:90:GLU:HG2	2:H:90:GLU:O	2.04	0.55
2:F:5[A]:GLY:N	2:F:6[A]:PRO:HD3	2.21	0.55
1:E:91:GLN:HB2	2:F:31:PHE:O	2.06	0.55
1:E:79:ARG:HD2	1:E:119:ALA:OXT	2.05	0.55
2:D:21:ASN:ND2	2:D:21:ASN:C	2.58	0.55
1:C:101:SER:O	1:C:102:ASP:CB	2.54	0.55
1:E:26:TYR:OH	1:E:81:HIS:HE1	1.89	0.55
1:E:44:ARG:HH11	1:E:44:ARG:CB	2.20	0.55
2:B:10:ASN:HB2	3:B:229:HOH:O	2.05	0.55
2:D:159:GLU:HA	2:D:162:GLU:OE1	2.06	0.55
1:C:89:GLY:O	1:C:91:GLN:N	2.40	0.54
1:G:2:ALA:HA	1:G:6:GLU:OE1	2.07	0.54
2:B:74:LYS:HD3	2:B:78:GLU:OE1	2.08	0.54
1:A:59:ASN:ND2	1:A:62:LEU:H	2.06	0.54
2:F:11[A]:VAL:HG12	2:F:12[A]:THR:N	2.22	0.54
2:F:73:ARG:HG2	2:F:74:LYS:N	2.22	0.54
2:B:31:PHE:CD2	2:B:37:VAL:HG21	2.43	0.54
1:C:44:ARG:HD2	2:D:13:GLU:OE1	2.08	0.54
1:E:13:LYS:HA	1:E:13:LYS:HE2	1.90	0.54
2:F:166:ARG:HG3	2:F:167:ARG:HD2	1.90	0.53
1:E:44:ARG:HB3	2:F:11[A]:VAL:HG11	1.91	0.53
2:H:114:LYS:HE2	2:H:142:ASN:ND2	2.23	0.53
2:B:22:THR:HG21	3:B:231:HOH:O	2.07	0.53
1:E:44:ARG:HB3	1:E:44:ARG:HH11	1.74	0.53
1:A:37:ARG:HH22	1:E:16:THR:HG21	1.73	0.53
2:D:94:GLU:N	2:D:94:GLU:OE1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:94:THR:HG22	1:E:109:ILE:CD1	2.39	0.53
1:G:94:THR:HG21	2:H:39:PHE:CZ	2.43	0.53
1:G:94:THR:HG21	2:H:39:PHE:HZ	1.73	0.53
2:F:73:ARG:CG	2:F:74:LYS:H	2.15	0.53
2:D:44:GLN:HE21	2:D:104:GLY:N	2.07	0.52
1:G:64:ASN:HB2	3:G:667:HOH:O	2.09	0.52
2:H:10[B]:ASN:OD1	2:H:11[B]:VAL:N	2.43	0.52
2:F:161:GLU:HG3	2:F:162:GLU:OE2	2.10	0.52
1:C:8:ASP:HB3	1:C:105:SER:HB3	1.92	0.52
1:C:7:LEU:HD21	1:C:106:LEU:HG	1.91	0.51
1:E:19:TRP:CD1	1:E:112:GLN:HB3	2.45	0.51
2:D:19:PRO:HB3	2:D:21:ASN:ND2	2.25	0.51
2:H:25:LYS:HD2	2:H:141:HIS:CE1	2.46	0.51
1:G:59:ASN:ND2	1:G:59:ASN:C	2.61	0.51
1:A:48:THR:OG1	1:A:51:ARG:HB3	2.11	0.51
2:F:153:ARG:HB3	2:F:153:ARG:NH1	2.26	0.51
2:D:79:ALA:HA	2:D:82:LYS:HG3	1.93	0.51
1:C:26:TYR:OH	1:C:81:HIS:HE1	1.93	0.51
1:C:48:THR:CG2	2:D:9:GLN:HG2	2.41	0.50
2:B:92:ARG:HG3	2:B:92:ARG:HH11	1.76	0.50
2:B:93:PRO:HA	2:B:96:GLN:HG3	1.93	0.50
2:D:158:GLU:O	2:D:162:GLU:HG3	2.11	0.50
2:D:131:PRO:HB2	1:E:35:SER:HB2	1.92	0.50
1:G:46:ALA:CA	2:H:11[A]:VAL:HG23	2.41	0.50
2:B:21:ASN:OD1	2:F:132:ASP:N	2.45	0.50
1:C:8:ASP:OD1	1:C:10:THR:HG23	2.12	0.50
2:D:21:ASN:O	2:D:22:THR:HB	2.11	0.50
2:B:21:ASN:ND2	3:B:253:HOH:O	2.45	0.50
2:D:90:GLU:C	2:D:164:TRP:HE1	2.15	0.50
2:B:22:THR:O	2:B:22:THR:HG23	2.12	0.50
2:F:11[A]:VAL:CG1	2:F:12[A]:THR:N	2.75	0.49
1:A:51:ARG:NH1	1:A:53:GLU:HB2	2.27	0.49
2:B:19:PRO:HB3	2:B:21:ASN:ND2	2.27	0.49
2:F:31:PHE:CD2	2:F:37:VAL:HG21	2.47	0.49
1:C:61:ASP:O	1:C:65:ILE:HG13	2.12	0.49
1:A:59:ASN:C	1:A:59:ASN:HD22	2.17	0.49
2:D:91:PHE:HB3	2:D:96:GLN:NE2	2.28	0.49
2:H:86:ILE:HG13	2:H:86:ILE:O	2.12	0.49
2:F:91:PHE:CE2	2:F:164:TRP:HA	2.48	0.48
1:C:89:GLY:C	1:C:91:GLN:H	2.16	0.48
2:F:51:LEU:O	2:F:54:LYS:HG3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:VAL:HG22	1:A:88:VAL:O	2.12	0.48
2:H:11[A]:VAL:HG22	2:H:12[A]:THR:H	1.79	0.48
2:B:83:LYS:HD2	2:B:83:LYS:N	2.28	0.48
1:A:22:LYS:HB3	1:A:115:GLU:HG3	1.95	0.48
2:F:162:GLU:N	2:F:162:GLU:OE1	2.47	0.48
1:C:57:THR:HG23	1:C:78:PRO:O	2.14	0.48
2:F:166:ARG:CG	2:F:167:ARG:HD2	2.44	0.47
2:H:43:ASN:HB2	2:H:44:GLN:NE2	2.29	0.47
2:B:120:GLU:N	2:B:120:GLU:OE1	2.46	0.47
2:H:56:ILE:CG1	2:H:57:TYR:H	2.26	0.47
1:G:44:ARG:NH2	3:G:688:HOH:O	2.39	0.47
1:G:22:LYS:HE2	1:G:115:GLU:OE2	2.14	0.47
1:C:94:THR:OG1	2:D:29:MET:HB3	2.14	0.47
1:G:44:ARG:HG3	2:H:11[B]:VAL:CG1	2.45	0.47
1:C:48:THR:HG22	2:D:9:GLN:HG2	1.97	0.46
2:B:28:ILE:HD11	2:B:126:ILE:HD11	1.97	0.46
1:C:15:ASN:ND2	3:C:162:HOH:O	2.48	0.46
1:C:25:LYS:NZ	2:D:123:SER:HB3	2.30	0.46
1:A:59:ASN:ND2	1:A:62:LEU:HD13	2.19	0.46
2:D:47:LEU:HG	2:D:98:TRP:CE3	2.51	0.46
2:B:101:ARG:HG2	2:B:109:LYS:HG2	1.99	0.45
1:E:37:ARG:NH2	3:E:540:HOH:O	2.49	0.45
1:G:22:LYS:CE	1:G:115:GLU:OE2	2.64	0.45
1:E:25:LYS:O	1:E:29:GLN:HG3	2.16	0.45
2:B:75:LEU:O	2:B:78:GLU:HB3	2.16	0.45
1:A:7:LEU:HD21	1:A:106:LEU:HG	1.98	0.45
2:F:55:LYS:O	2:F:55:LYS:HD2	2.16	0.45
2:D:56:ILE:HG22	2:D:89:LYS:O	2.17	0.45
1:G:115:GLU:OE1	1:G:117:ARG:NE	2.50	0.45
2:B:19:PRO:HB3	2:B:21:ASN:HD21	1.82	0.45
2:D:56:ILE:O	2:D:56:ILE:HG23	2.18	0.44
1:C:99:SER:HA	2:D:23:THR:O	2.17	0.44
2:D:63:PRO:HG3	3:D:292:HOH:O	2.16	0.44
1:C:77:ALA:HA	1:C:78:PRO:HD3	1.60	0.44
2:F:38:ASN:ND2	2:F:41:THR:HG23	2.32	0.44
1:A:84:VAL:CG2	1:A:117:ARG:HE	2.24	0.44
1:G:46:ALA:HA	2:H:11[A]:VAL:HG23	2.00	0.44
2:H:10[B]:ASN:O	2:H:11[B]:VAL:CG2	2.66	0.43
2:H:27:ASN:OD1	2:H:141:HIS:HB3	2.19	0.43
2:H:61:GLU:HA	2:H:83:LYS:O	2.18	0.43
2:F:161:GLU:HG3	2:F:162:GLU:CD	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:LEU:N	1:A:62:LEU:HD12	2.34	0.43
1:C:9:LEU:HD22	1:C:106:LEU:HD12	2.01	0.43
1:E:26:TYR:OH	1:E:81:HIS:CE1	2.72	0.43
1:A:70:GLY:O	1:A:71:LYS:O	2.37	0.43
1:C:96:PHE:HB3	1:C:106:LEU:HD23	2.00	0.43
2:D:165:GLU:OE1	2:D:165:GLU:HA	2.19	0.43
2:H:51:LEU:HD23	2:H:96:GLN:HG2	2.01	0.43
2:H:81:ARG:HH11	2:H:81:ARG:HG2	1.84	0.43
2:D:56:ILE:CG2	2:D:89:LYS:HB2	2.48	0.42
2:F:73:ARG:CG	2:F:74:LYS:N	2.81	0.42
2:B:92:ARG:HG3	2:B:92:ARG:NH1	2.33	0.42
2:F:38:ASN:HD22	2:F:41:THR:HG23	1.84	0.42
2:H:78:GLU:HG2	2:H:78:GLU:O	2.19	0.42
2:F:102:VAL:O	2:F:107:GLY:HA3	2.20	0.42
2:D:53:ASN:ND2	2:D:155:LEU:HD12	2.33	0.42
1:C:84:VAL:HG21	1:C:117:ARG:NE	2.33	0.42
2:D:131:PRO:CB	1:E:35:SER:HB2	2.50	0.42
1:G:44:ARG:CG	2:H:11[A]:VAL:HG21	2.47	0.42
2:D:46:ARG:HH21	2:D:46:ARG:HG2	1.85	0.42
1:C:91:GLN:HB2	2:D:31:PHE:O	2.20	0.42
1:C:79:ARG:NH2	1:C:119:ALA:O	2.53	0.42
2:D:74:LYS:HE3	2:D:77:GLU:OE2	2.20	0.42
2:D:165:GLU:O	2:D:168:ASN:O	2.37	0.41
1:G:79:ARG:HA	1:G:79:ARG:HD3	1.65	0.41
1:A:97:THR:HG23	1:A:107:GLU:HG3	2.01	0.41
1:G:44:ARG:CG	2:H:11[B]:VAL:HG11	2.48	0.41
2:H:82:LYS:HB2	2:H:84:TYR:HE1	1.85	0.41
1:C:67:ASP:O	1:C:68:ILE:C	2.58	0.41
1:A:48:THR:HG21	2:B:6:PRO:HG3	2.02	0.41
2:F:162:GLU:N	2:F:162:GLU:CD	2.74	0.41
2:B:20:LYS:HE2	3:B:250:HOH:O	2.20	0.41
2:D:91:PHE:CG	2:D:164:TRP:HD1	2.39	0.41
1:E:33:LYS:NZ	3:E:400:HOH:O	2.54	0.41
1:A:18:VAL:CG1	2:B:128:THR:HG22	2.51	0.41
1:A:59:ASN:HD21	1:A:62:LEU:CD1	2.20	0.41
1:E:48:THR:HG23	1:E:51:ARG:HB2	2.02	0.41
1:E:25:LYS:HD3	3:F:181:HOH:O	2.21	0.41
1:G:45:ILE:O	2:H:11[A]:VAL:CG2	2.69	0.41
1:G:3:GLU:O	1:G:6:GLU:HB3	2.20	0.41
1:C:26:TYR:O	1:C:30:GLN:HG3	2.21	0.41
2:B:27:ASN:HD22	2:B:142:ASN:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:147:THR:OG1	2:H:152:HIS:HE1	2.04	0.40
1:E:68:ILE:HD11	2:H:135:PHE:CE2	2.56	0.40
2:B:105:LYS:HD3	3:B:201:HOH:O	2.20	0.40
1:A:37:ARG:NH1	1:A:37:ARG:HG3	2.34	0.40
2:B:78:GLU:O	2:B:78:GLU:HG2	2.20	0.40
1:A:106:LEU:HA	1:A:106:LEU:HD23	1.93	0.40
2:H:42:TRP:CH2	2:H:100:LEU:HD21	2.56	0.40
1:E:44:ARG:NH1	1:E:44:ARG:HB3	2.35	0.40
1:E:88:VAL:O	1:E:88:VAL:HG13	2.21	0.40
2:B:90:GLU:N	2:B:90:GLU:CD	2.72	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	116/118 (98%)	105 (90%)	6 (5%)	5 (4%)	3	0
1	C	116/118 (98%)	103 (89%)	7 (6%)	6 (5%)	2	0
1	E	116/118 (98%)	114 (98%)	2 (2%)	0	100	100
1	G	116/118 (98%)	109 (94%)	7 (6%)	0	100	100
2	B	135/171 (79%)	128 (95%)	5 (4%)	2 (2%)	13	2
2	D	149/171 (87%)	139 (93%)	8 (5%)	2 (1%)	15	2
2	F	153/171 (90%)	140 (92%)	7 (5%)	6 (4%)	4	0
2	H	136/171 (80%)	121 (89%)	10 (7%)	5 (4%)	4	0
All	All	1037/1156 (90%)	959 (92%)	52 (5%)	26 (2%)	7	1

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	PRO
1	A	76	SER
2	B	119	THR
1	C	102	ASP
2	F	77	GLU
2	F	79	ALA
2	F	117	GLY
2	F	118	VAL
2	F	155	LEU
1	C	68	ILE
1	C	79	ARG
1	C	90	GLY
1	A	68	ILE
1	C	76	SER
2	D	22	THR
2	H	104	GLY
2	H	120	GLU
1	A	71	LYS
2	B	89	LYS
1	C	8	ASP
2	F	80	ARG
2	H	57	TYR
1	A	75	VAL
2	D	36	LYS
2	H	60	GLU
2	H	56	ILE

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	96/96 (100%)	94 (98%)	2 (2%)	61	42
1	C	95/96 (99%)	94 (99%)	1 (1%)	80	69
1	E	96/96 (100%)	92 (96%)	4 (4%)	36	14
1	G	96/96 (100%)	92 (96%)	4 (4%)	36	14
2	B	122/147 (83%)	117 (96%)	5 (4%)	37	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	135/147 (92%)	131 (97%)	4 (3%)	48	26
2	F	138/147 (94%)	130 (94%)	8 (6%)	25	8
2	H	124/147 (84%)	118 (95%)	6 (5%)	31	12
All	All	902/972 (93%)	868 (96%)	34 (4%)	40	17

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	117	ARG
2	B	21	ASN
2	B	59	GLU
2	B	83	LYS
2	B	90	GLU
2	B	95	ASP
1	C	3	GLU
2	D	21	ASN
2	D	38	ASN
2	D	108	ARG
2	D	121	ASN
1	E	13	LYS
1	E	27	LEU
1	E	44	ARG
1	E	48	THR
2	F	21	ASN
2	F	55	LYS
2	F	90	GLU
2	F	94	GLU
2	F	96	GLN
2	F	99	LEU
2	F	153	ARG
2	F	161	GLU
1	G	35	SER
1	G	59	ASN
1	G	67	ASP
1	G	88	VAL
2	H	44	GLN
2	H	57	TYR
2	H	74	LYS
2	H	91	PHE
2	H	92	ARG

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Mol	Chain	Res	Type
2	H	96	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	30	GLN
1	A	59	ASN
2	B	27	ASN
2	B	43	ASN
2	B	58	GLN
2	B	129	GLN
2	B	141	HIS
2	B	142	ASN
1	C	15	ASN
1	C	30	GLN
1	C	81	HIS
2	D	21	ASN
2	D	38	ASN
2	D	44	GLN
2	D	53	ASN
1	E	81	HIS
1	E	86	GLN
2	F	38	ASN
2	F	96	GLN
2	F	129	GLN
1	G	59	ASN
1	G	81	HIS
1	G	91	GLN
2	H	58	GLN
2	H	121	ASN
2	H	142	ASN
2	H	152	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	118/118 (100%)	0.75	10 (8%)	13	14	22, 39, 69, 80	6 (5%)
1	C	118/118 (100%)	1.24	28 (23%)	1	1	29, 52, 76, 85	8 (6%)
1	E	118/118 (100%)	0.66	7 (5%)	26	27	20, 32, 58, 75	0
1	G	118/118 (100%)	1.06	17 (14%)	3	4	21, 42, 69, 77	1 (0%)
2	B	135/171 (78%)	0.86	16 (11%)	6	7	21, 42, 68, 82	0
2	D	151/171 (88%)	1.04	28 (18%)	2	2	27, 49, 72, 79	0
2	F	145/171 (84%)	1.05	24 (16%)	2	2	19, 38, 70, 78	10 (6%)
2	H	133/171 (77%)	1.41	32 (24%)	1	1	25, 48, 76, 83	10 (7%)
All	All	1036/1156 (89%)	1.01	162 (15%)	3	3	19, 42, 73, 85	35 (3%)

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	164	TRP	10.3
2	H	55	LYS	10.1
2	D	91	PHE	10.1
1	G	75	VAL	8.6
1	A	74	SER	8.0
1	C	73	ALA	8.0
2	H	7[A]	SER	7.9
1	E	88	VAL	7.8
1	G	73	ALA	7.7
1	A	75	VAL	7.7
2	B	91	PHE	7.1
2	B	21	ASN	6.9
2	H	56	ILE	6.8
2	F	161	GLU	6.8
2	F	160	ALA	6.5
2	B	56	ILE	6.5

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Mol	Chain	Res	Type	RSRZ
2	B	90	GLU	6.5
1	C	77	ALA	6.1
1	C	68	ILE	6.1
2	H	91	PHE	5.8
2	F	163	GLU	5.8
1	G	88	VAL	5.5
1	C	69	GLY	5.3
2	D	92	ARG	5.3
2	H	57	TYR	5.2
2	F	91	PHE	5.2
2	H	10[A]	ASN	5.2
2	H	8[A]	SER	5.0
2	B	54	LYS	5.0
1	E	49	GLN	5.0
1	C	70	GLY	4.7
1	G	119	ALA	4.7
2	H	88	LEU	4.7
2	H	90	GLU	4.7
2	D	107	GLY	4.6
2	F	167	ARG	4.5
1	G	74	SER	4.5
1	E	119	ALA	4.5
2	H	9[A]	GLN	4.5
2	D	21	ASN	4.5
2	D	168	ASN	4.5
2	F	8[A]	SER	4.3
2	B	76	ARG	4.3
2	D	164	TRP	4.2
1	G	76	SER	4.2
2	F	7[A]	SER	4.2
2	H	54	LYS	4.2
2	H	86	ILE	4.2
2	F	168	ASN	4.2
2	D	40	ALA	4.1
1	G	70	GLY	4.1
2	H	11[A]	VAL	4.0
1	G	72	PRO	4.0
2	H	62	MET	3.9
1	C	49	GLN	3.9
2	B	92	ARG	3.9
2	F	153	ARG	3.9
1	C	100	SER	3.8

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Mol	Chain	Res	Type	RSRZ
2	F	6[A]	PRO	3.8
2	H	84	TYR	3.8
1	C	72	PRO	3.8
2	D	23	THR	3.8
2	D	154	THR	3.8
2	B	86	ILE	3.7
1	C	88	VAL	3.7
2	D	163	GLU	3.7
2	F	80	ARG	3.7
2	F	10[A]	ASN	3.7
1	E	48	THR	3.7
2	B	23	THR	3.6
2	D	162	GLU	3.6
1	A	72	PRO	3.6
1	G	2	ALA	3.6
1	C	119	ALA	3.6
1	A	88	VAL	3.5
1	C	104	LEU	3.5
2	D	157	ALA	3.5
1	G	77	ALA	3.5
2	H	93	PRO	3.5
2	B	6	PRO	3.4
2	H	77	GLU	3.4
2	F	5[A]	GLY	3.4
1	G	90	GLY	3.3
2	H	52	SER	3.3
1	E	50	GLY	3.3
1	A	49	GLN	3.3
1	C	75	VAL	3.2
2	D	166	ARG	3.2
2	H	60	GLU	3.2
2	H	58	GLN	3.2
1	A	119	ALA	3.2
2	B	55	LYS	3.2
1	C	67	ASP	3.2
2	F	117	GLY	3.2
1	C	102	ASP	3.1
2	F	90	GLU	3.1
2	B	88	LEU	3.1
2	F	9[A]	GLN	3.1
2	D	159	GLU	3.0
1	E	36	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	71	LYS	3.0
1	C	7	LEU	3.0
1	C	9	LEU	3.0
1	G	66	HIS	3.0
2	D	22	THR	3.0
1	C	36	GLY	2.9
2	D	161	GLU	2.9
2	H	78	GLU	2.8
1	G	67	ASP	2.8
2	D	160	ALA	2.7
2	D	155	LEU	2.7
1	C	26	TYR	2.7
2	F	89	LYS	2.7
1	G	64	ASN	2.7
2	F	11[A]	VAL	2.7
2	H	59	GLU	2.6
1	C	109	ILE	2.6
2	H	95	ASP	2.6
1	A	73	ALA	2.6
2	D	158	GLU	2.6
2	B	22	THR	2.6
2	D	41	THR	2.5
2	D	105	LYS	2.5
2	D	39	PHE	2.5
2	H	80	ARG	2.5
2	H	87	VAL	2.5
2	H	102	VAL	2.5
2	H	99	LEU	2.5
2	F	166	ARG	2.4
1	C	2	ALA	2.4
1	G	109	ILE	2.4
1	E	110	VAL	2.4
2	F	159	GLU	2.3
2	F	82	LYS	2.3
1	A	109	ILE	2.3
1	C	30	GLN	2.3
1	C	38	GLY	2.3
2	H	92	ARG	2.3
1	A	70	GLY	2.2
2	D	34	ALA	2.2
1	C	90	GLY	2.2
2	H	51	LEU	2.2

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Full wwPDB X-ray Structure Validation Report

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Mol	Chain	Res	Type	RSRZ
1	C	89	GLY	2.2
2	D	46	ARG	2.2
2	H	38	ASN	2.1
1	C	4	ARG	2.1
2	H	98	TRP	2.1
1	A	56	PHE	2.1
2	B	96	GLN	2.1
2	D	36	LYS	2.1
1	C	15	ASN	2.1
2	F	75	LEU	2.1
2	H	79	ALA	2.0
2	B	149	LEU	2.0
2	B	94	GLU	2.0
2	D	116	GLY	2.0
1	G	63	ALA	2.0
2	F	162	GLU	2.0
1	C	64	ASN	2.0
2	D	121	ASN	2.0
1	C	106	LEU	2.0
2	D	99	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.