Full wwPDB X-ray Structure Validation Report (i)

May 21, 2020 – 02:02 pm BST

PDB ID	:	2D31
Title	:	Crystal structure of disulfide-linked HLA-G dimer
Authors	:	Shiroishi, M.; Kuroki, K.; Ose, T.; Rasubala, L.; Shiratori, I.; Arase, H.; Tsumoto, K.; Kumagai, I.; Kohda, D.; Maenaka, K.
Deposited on	:	2005-09-23
Resolution	:	3.20 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 following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

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 3.20 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.
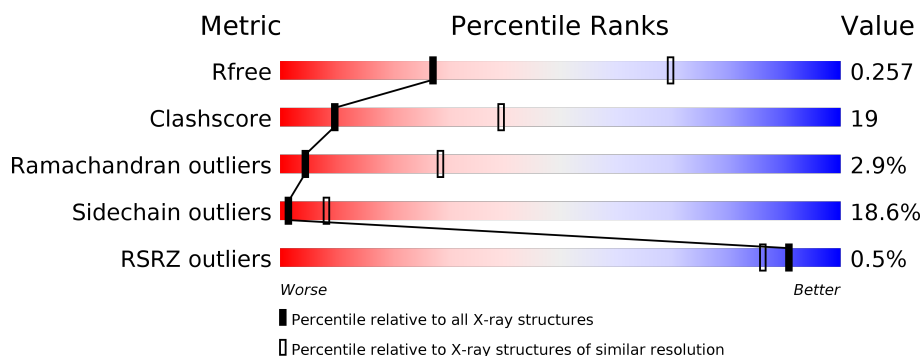
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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	276	50% 40% 8% ·
1	D	276	% 55% 31% 9% 5%
2	B	100	50% 39% 10% ·
2	E	100	% 45% 44% 10% ·
3	C	9	44% 22% 22% 11%
3	F	9	44% 33% 22%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6124 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 HLA class I histocompatibility antigen, alpha chain G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total 2181	C 1358	N 394	O 416	S 13	0	0	0
1	D	262	Total 2123	C 1324	N 382	O 404	S 13	0	0	0

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total 829	C 528	N 140	O 158	S 3	0	0	0
2	E	99	Total 829	C 528	N 140	O 158	S 3	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
E	0	MET	-	initiating methionine	UNP P61769

- Molecule 3 is a protein called 9-mer peptide from Histone H2A.

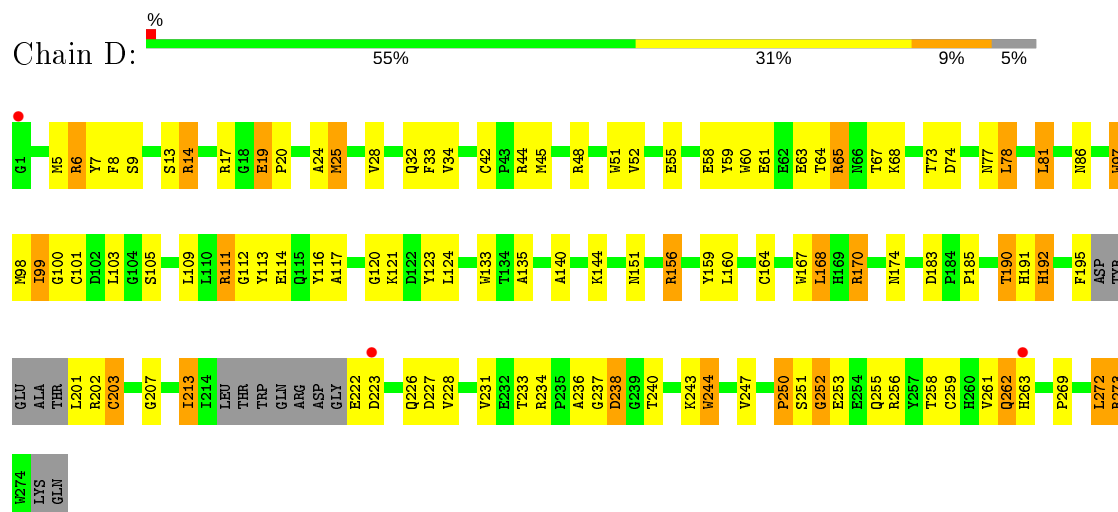| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total 81	C 52	N 18	O 11	0	0	0
3	F	9	Total 81	C 52	N 18	O 11	0	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: HLA class I histocompatibility antigen, alpha chain G
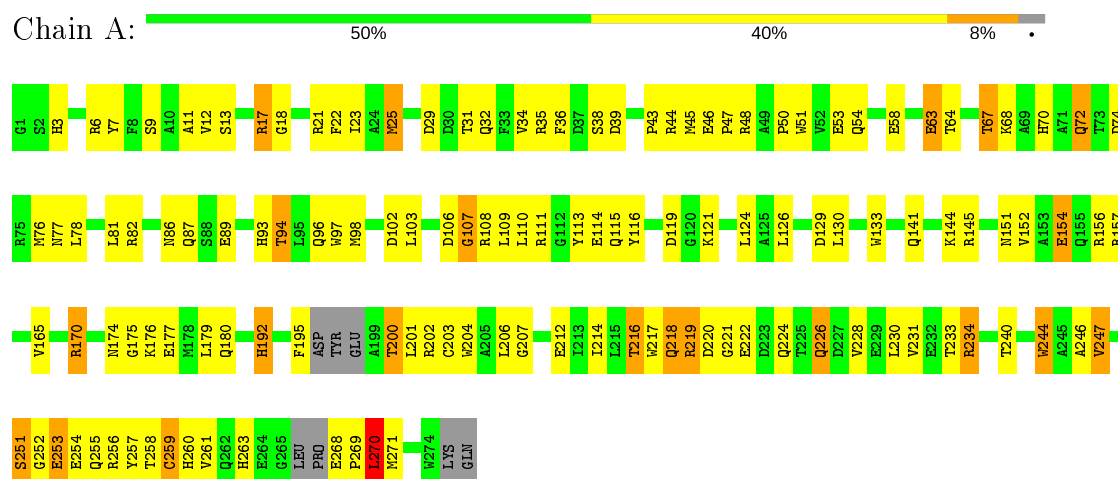
- Molecule 1: HLA class I histocompatibility antigen, alpha chain G

- Molecule 2: Beta-2-microglobulin

MET I1 I7 Q8 V9 Y10 S11 R12 H13 E16 N17 N21 F22 L23 N24 C25 Y26 V27 S33 D34 I35 L39 R45 K48 V49 E50 H51 S52 D53 L54 S55 F56 S57 K58 D59 W60 S61 F62 Y63 L64 L65 Y66 Y67 F70 T71 P72 R81 V82 N83 H84 V85

T86 L87 S88 Q89 P90 K91 I92 D96 R97 D98 M99

• Molecule 2: Beta-2-microglobulin

Chain E:

%

45% 44% 10%

MET I1 T4 Q8 V9 Y10 S11 R12 H13 P14 K19 S20 N21 F22 L23 N24 C25 Y26 V27 S28 G29 F30 H31 D34 I35 E36 V37 D38 L39 L40 K41 R45 I46 E47 K48 V49 S52 D53 L54 S55 F56 W60 S61 L65 T68 E69 F70 T71 P72 T73 E74

K75 Y78 A79 C80 R81 V82 N83 H84 V85 T86 L87 S88 Q89 I92 V93 D98 M99

• Molecule 3: 9-mer peptide from Histone H2A

Chain C:

44% 22% 22% 11%

R1 I2 I3 P4 R5 H6 L7 Q8 L9

• Molecule 3: 9-mer peptide from Histone H2A

Chain F:

44% 33% 22%

R1 R5 H6 L7 Q8 L9

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	94.64Å 127.81Å 72.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 47.96 – 3.00	Depositor EDS
% Data completeness (in resolution range)	83.8 (50.00-3.20) 83.5 (47.96-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.94 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.235 , 0.298 0.235 , 0.257	Depositor DCC
R_{free} test set	1100 reflections (7.26%)	wwPDB-VP
Wilson B-factor (Å^2)	56.7	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 25.6	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	6124	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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 ⓘ

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	0.51	0/2238	0.67	1/3034 (0.0%)
1	D	0.53	0/2179	0.68	0/2954
2	B	0.50	0/852	0.70	1/1152 (0.1%)
2	E	0.62	0/852	0.68	0/1152
3	C	0.52	0/82	1.01	1/108 (0.9%)
3	F	0.49	0/82	0.74	0/108
All	All	0.53	0/6285	0.68	3/8508 (0.0%)

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	270	LEU	CA-CB-CG	6.68	130.66	115.30
3	C	7	LEU	CA-CB-CG	6.56	130.38	115.30
2	B	87	LEU	CA-CB-CG	5.27	127.42	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2181	0	2037	94	0
1	D	2123	0	1987	84	0
2	B	829	0	794	34	0
2	E	829	0	794	41	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	81	0	94	5	0
3	F	81	0	94	7	0
All	All	6124	0	5800	230	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 19.

All (230) 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:31:THR:HG21	1:A:51:TRP:HH2	1.31	0.96
1:A:219:ARG:HG3	1:A:220:ASP:H	1.33	0.92
1:A:110:LEU:HD22	1:A:111:ARG:HE	1.38	0.87
1:D:213:ILE:HG22	1:D:263:HIS:CE1	2.10	0.86
1:A:32:GLN:NE2	1:A:48:ARG:HE	1.75	0.84
1:A:218:GLN:HG2	1:A:258:THR:O	1.78	0.82
1:A:93:HIS:HD2	1:A:119:ASP:OD1	1.61	0.82
1:A:176:LYS:HA	1:A:180:GLN:HG3	1.63	0.79
1:D:185:PRO:HD3	1:D:263:HIS:HD2	1.49	0.78
1:A:31:THR:HG21	1:A:51:TRP:CH2	2.18	0.77
1:A:108:ARG:HD2	1:A:109:LEU:HD23	1.69	0.75
1:A:63:GLU:O	1:A:67:THR:HG23	1.86	0.75
1:A:12:VAL:HG22	1:A:94:THR:HB	1.67	0.75
1:A:218:GLN:CG	1:A:258:THR:HG23	2.17	0.74
2:E:13:HIS:O	2:E:21:ASN:ND2	2.20	0.74
1:D:244:TRP:CH2	2:E:99:MET:HA	2.23	0.74
1:D:244:TRP:HH2	2:E:99:MET:HA	1.53	0.73
1:D:185:PRO:HD3	1:D:263:HIS:CD2	2.23	0.72
2:B:7:ILE:HG12	2:B:82:VAL:HG11	1.71	0.72
2:B:96:ASP:HB3	2:B:99:MET:HB3	1.71	0.72
1:A:216:THR:O	1:A:259:CYS:HA	1.92	0.70
1:D:123:TYR:CZ	1:D:140:ALA:HA	2.28	0.69
1:D:7:TYR:O	1:D:98:MET:HA	1.93	0.68
1:A:25:MET:HB3	1:A:35:ARG:HG3	1.76	0.68
1:D:207:GLY:HA2	1:D:240:THR:HB	1.76	0.68
1:A:218:GLN:HG2	1:A:258:THR:HG23	1.76	0.67
1:A:46:GLU:HB2	1:A:47:PRO:HD2	1.74	0.67
2:B:45:ARG:NE	2:B:81:ARG:HH12	1.91	0.67
1:A:74:ASP:HA	1:A:77:ASN:HB2	1.76	0.67
2:E:41:LYS:HD2	2:E:78:TYR:CE1	2.30	0.67
1:A:51:TRP:CE2	1:A:179:LEU:HD21	2.30	0.66

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:HG3	1:A:246:ALA:HB2	1.78	0.65
1:D:203:CYS:O	1:D:244:TRP:HB2	1.97	0.65
1:A:228:VAL:HG12	1:A:247:VAL:HG13	1.77	0.65
2:B:12:ARG:HG3	2:B:22:PHE:HB2	1.78	0.64
1:A:103:LEU:HD22	1:A:107:GLY:O	1.97	0.64
1:A:218:GLN:HG3	1:A:258:THR:HG23	1.79	0.64
1:A:3:HIS:HD2	1:A:29:ASP:OD2	1.79	0.64
1:D:32:GLN:HE22	1:D:48:ARG:HH11	1.46	0.63
2:B:34:ASP:O	2:B:84:HIS:HD2	1.82	0.63
1:A:110:LEU:HD13	1:A:111:ARG:HH11	1.62	0.62
1:A:6:ARG:CZ	1:A:113:TYR:OH	2.47	0.62
1:D:14:ARG:HG3	1:D:17:ARG:CZ	2.30	0.62
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.80	0.62
2:E:37:VAL:HG22	2:E:82:VAL:HG22	1.82	0.61
2:B:13:HIS:H	2:B:21:ASN:HD21	1.48	0.61
1:D:234:ARG:HD2	2:E:26:TYR:CZ	2.35	0.61
1:D:48:ARG:HH12	2:E:53:ASP:CG	2.05	0.61
1:D:244:TRP:C	1:D:244:TRP:CD1	2.73	0.60
2:E:27:VAL:HG23	2:E:30:PHE:CE2	2.36	0.60
1:A:219:ARG:HG3	1:A:220:ASP:N	2.13	0.60
1:A:38:SER:HA	1:A:43:PRO:HB3	1.83	0.60
2:B:17:ASN:HA	2:B:72:PRO:O	2.01	0.60
1:D:44:ARG:HH22	1:D:60:TRP:HB3	1.66	0.60
2:E:92:ILE:HD12	2:E:92:ILE:C	2.22	0.60
1:A:9:SER:OG	1:A:22:PHE:CZ	2.54	0.59
3:C:3:ILE:HG13	3:C:4:PRO:HD2	1.82	0.59
1:D:244:TRP:HH2	2:E:99:MET:HG2	1.68	0.59
1:D:258:THR:HG22	1:D:273:ARG:HB3	1.84	0.59
2:E:74:GLU:N	2:E:74:GLU:OE1	2.37	0.58
1:A:89:GLU:CD	1:A:89:GLU:H	2.07	0.58
1:A:17:ARG:HG3	1:A:18:GLY:H	1.68	0.58
1:A:207:GLY:HA2	1:A:240:THR:HB	1.85	0.58
2:B:48:LYS:HD2	2:B:48:LYS:H	1.68	0.58
1:D:33:PHE:HB2	1:D:52:VAL:HG21	1.86	0.58
1:A:234:ARG:HH21	2:B:8:GLN:NE2	2.02	0.58
2:B:51:HIS:HA	2:B:66:TYR:HA	1.84	0.58
1:D:170:ARG:HD2	1:D:174:ASN:HD21	1.67	0.58
1:D:236:ALA:HB1	2:E:12:ARG:HD3	1.85	0.57
1:D:243:LYS:HG3	1:D:244:TRP:N	2.19	0.57
2:E:29:GLY:HA2	2:E:61:SER:HB2	1.86	0.57
1:A:50:PRO:HA	1:A:53:GLU:OE1	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:LEU:HD11	1:D:123:TYR:CZ	2.40	0.56
2:E:79:ALA:HB1	2:E:92:ILE:CD1	2.35	0.56
1:A:6:ARG:NE	1:A:113:TYR:OH	2.39	0.56
1:A:17:ARG:HG3	1:A:18:GLY:N	2.20	0.56
1:A:12:VAL:HA	1:A:93:HIS:O	2.06	0.56
1:D:262:GLN:C	1:D:263:HIS:HD1	2.09	0.55
1:D:5:MET:HB2	1:D:168:LEU:HG	1.88	0.55
1:A:219:ARG:HA	1:A:257:TYR:CE2	2.41	0.55
1:A:207:GLY:HA2	1:A:240:THR:CB	2.37	0.55
1:D:100:GLY:HA3	1:D:113:TYR:CZ	2.42	0.55
1:D:213:ILE:HD12	1:D:243:LYS:HB3	1.88	0.55
1:A:21:ARG:HG3	1:A:39:ASP:OD1	2.07	0.55
2:E:8:GLN:HB3	2:E:26:TYR:HD2	1.72	0.55
1:A:17:ARG:CG	1:A:18:GLY:H	2.20	0.54
1:D:8:PHE:HB3	2:E:56:PHE:CE1	2.42	0.54
1:D:97:TRP:HZ3	1:D:114:GLU:CD	2.10	0.54
1:A:244:TRP:C	1:A:244:TRP:CD1	2.81	0.54
1:D:32:GLN:NE2	1:D:48:ARG:HH11	2.05	0.54
1:D:244:TRP:CH2	2:E:99:MET:HG2	2.43	0.54
1:D:81:LEU:HD11	1:D:123:TYR:OH	2.08	0.54
1:A:93:HIS:CD2	1:A:119:ASP:OD1	2.52	0.54
1:D:111:ARG:HD3	1:D:112:GLY:H	1.73	0.54
2:B:96:ASP:HB3	2:B:99:MET:CB	2.38	0.53
1:A:72:GLN:HE21	1:A:72:GLN:HA	1.73	0.53
1:A:9:SER:HB3	1:A:97:TRP:HE3	1.74	0.53
1:D:9:SER:HG	1:D:97:TRP:HE1	1.55	0.53
2:E:84:HIS:ND1	2:E:86:THR:HG22	2.23	0.53
1:D:191:HIS:HA	1:D:201:LEU:HD23	1.90	0.53
1:D:8:PHE:CD2	1:D:98:MET:HB3	2.43	0.52
1:A:156:ARG:CZ	3:C:7:LEU:HD12	2.39	0.52
1:D:234:ARG:HD3	2:E:8:GLN:NE2	2.24	0.52
2:E:46:ILE:O	2:E:46:ILE:HG13	2.08	0.52
1:A:114:GLU:OE2	1:A:156:ARG:HD2	2.09	0.52
1:D:97:TRP:HZ3	1:D:114:GLU:OE1	1.93	0.51
1:D:170:ARG:HD2	1:D:174:ASN:ND2	2.25	0.51
1:D:238:ASP:OD2	1:D:240:THR:OG1	2.28	0.51
1:D:167:TRP:CE2	3:F:1:ARG:HG3	2.45	0.51
2:B:56:PHE:HB2	2:B:61:SER:O	2.10	0.51
1:A:45:MET:SD	1:A:67:THR:HG21	2.51	0.51
2:E:24:ASN:HB3	2:E:65:LEU:HD11	1.92	0.51
1:A:51:TRP:CZ2	1:A:179:LEU:HD21	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4:THR:HA	2:E:86:THR:HG21	1.92	0.51
1:A:203:CYS:HB2	1:A:217:TRP:CZ2	2.45	0.51
1:D:202:ARG:NH2	2:E:98:ASP:O	2.44	0.51
1:A:256:ARG:HH21	1:A:256:ARG:HG2	1.76	0.50
1:D:6:ARG:HA	1:D:99:ILE:O	2.12	0.50
1:A:253:GLU:OE1	1:A:256:ARG:HB2	2.12	0.50
1:A:116:TYR:OH	3:C:7:LEU:HD13	2.12	0.49
1:D:74:ASP:HA	1:D:77:ASN:HB2	1.95	0.49
1:D:13:SER:HA	1:D:20:PRO:HB3	1.93	0.49
1:A:67:THR:O	1:A:70:HIS:HB2	2.13	0.49
2:B:33:SER:HB2	2:B:54:LEU:HD21	1.93	0.49
1:A:32:GLN:HE21	1:A:48:ARG:HE	1.56	0.49
1:D:64:THR:O	1:D:68:LYS:HB2	2.11	0.49
1:A:106:ASP:O	1:A:108:ARG:N	2.46	0.48
1:A:11:ALA:O	1:A:94:THR:HA	2.12	0.48
1:A:261:VAL:O	1:A:270:LEU:HD13	2.13	0.48
1:D:262:GLN:HE21	1:D:262:GLN:H	1.61	0.48
1:A:48:ARG:NH1	2:B:53:ASP:HB2	2.27	0.48
2:B:23:LEU:HD13	2:B:39:LEU:HD12	1.95	0.48
1:D:97:TRP:CZ2	1:D:99:ILE:HG12	2.49	0.48
1:D:28:VAL:HG11	1:D:51:TRP:CH2	2.49	0.48
1:A:204:TRP:HE3	1:A:206:LEU:HD21	1.77	0.48
1:A:130:LEU:HD23	1:A:157:ARG:HG3	1.95	0.48
1:D:120:GLY:HA2	2:E:31:HIS:CE1	2.49	0.48
1:A:70:HIS:CE1	3:C:6:HIS:ND1	2.82	0.47
1:A:23:ILE:HA	1:A:36:PHE:O	2.15	0.47
1:D:234:ARG:HD2	2:E:26:TYR:CE2	2.49	0.47
1:D:250:PRO:O	1:D:252:GLY:N	2.47	0.47
1:A:244:TRP:CZ3	2:B:99:MET:O	2.67	0.47
1:A:133:TRP:HB2	1:A:144:LYS:HG3	1.96	0.47
1:A:46:GLU:HB2	1:A:47:PRO:CD	2.42	0.47
1:A:234:ARG:HG3	2:B:10:TYR:CZ	2.49	0.47
1:A:114:GLU:OE1	1:A:156:ARG:NH2	2.48	0.46
1:D:8:PHE:HB3	2:E:56:PHE:CZ	2.51	0.46
2:B:51:HIS:HB3	2:B:66:TYR:CD2	2.51	0.46
2:B:81:ARG:HG3	2:B:92:ILE:HG12	1.97	0.46
3:F:1:ARG:HB3	3:F:1:ARG:HH21	1.81	0.46
2:B:12:ARG:HB2	2:B:22:PHE:HB2	1.98	0.46
1:A:3:HIS:CD2	1:A:29:ASP:OD2	2.65	0.46
1:A:244:TRP:CH2	2:B:99:MET:HG3	2.51	0.46
1:A:13:SER:HB3	1:A:78:LEU:HD13	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:TRP:HZ2	2:B:98:ASP:O	1.99	0.46
1:D:7:TYR:HB2	1:D:99:ILE:HG13	1.97	0.45
1:A:103:LEU:HD21	1:A:165:VAL:HG13	1.97	0.45
1:A:64:THR:O	1:A:68:LYS:HB2	2.16	0.45
2:E:49:VAL:HG12	2:E:68:THR:OG1	2.17	0.45
1:A:34:VAL:HG22	1:A:45:MET:CE	2.46	0.45
2:E:45:ARG:HH11	2:E:81:ARG:NH1	2.15	0.45
1:A:35:ARG:HB2	1:A:48:ARG:HD3	1.98	0.45
2:B:63:TYR:C	2:B:63:TYR:CD1	2.89	0.45
1:D:61:GLU:O	1:D:65:ARG:HB2	2.16	0.45
1:D:213:ILE:HD12	1:D:243:LYS:CB	2.47	0.45
1:D:190:THR:HB	1:D:192:HIS:NE2	2.32	0.45
2:E:10:TYR:CG	2:E:11:SER:N	2.84	0.45
1:A:212:GLU:O	1:A:263:HIS:HD2	2.00	0.45
1:A:3:HIS:HA	1:A:29:ASP:OD1	2.17	0.44
1:A:224:GLN:OE1	1:A:226:GLN:CG	2.65	0.44
2:B:49:VAL:HG23	2:B:67:TYR:O	2.16	0.44
2:B:34:ASP:O	2:B:84:HIS:CD2	2.65	0.44
1:D:33:PHE:HB2	1:D:52:VAL:CG2	2.47	0.44
1:A:175:GLY:HA3	1:A:179:LEU:HD23	1.98	0.44
2:E:36:GLU:HG3	2:E:83:ASN:HB3	2.00	0.44
1:A:170:ARG:HE	1:A:174:ASN:HD21	1.65	0.44
1:D:78:LEU:HA	1:D:78:LEU:HD13	1.86	0.44
2:E:23:LEU:HB2	2:E:70:PHE:CD2	2.53	0.44
2:E:92:ILE:HD12	2:E:93:VAL:N	2.33	0.44
1:D:6:ARG:HD2	1:D:8:PHE:CZ	2.53	0.44
1:A:9:SER:CB	1:A:97:TRP:HE3	2.30	0.43
2:B:27:VAL:HG11	2:B:35:ILE:HD11	2.00	0.43
1:A:228:VAL:HG12	1:A:247:VAL:CG1	2.47	0.43
1:A:253:GLU:HG3	1:A:253:GLU:O	2.19	0.43
2:B:59:ASP:O	2:B:61:SER:N	2.50	0.43
1:D:237:GLY:HA3	2:E:12:ARG:NE	2.34	0.43
1:D:73:THR:HG21	3:F:6:HIS:HB3	2.00	0.43
2:B:16:GLU:O	2:B:72:PRO:HG2	2.19	0.43
1:D:116:TYR:OH	3:F:7:LEU:HB2	2.19	0.43
1:A:151:ASN:O	1:A:154:GLU:HG2	2.19	0.42
1:D:19:GLU:HA	1:D:20:PRO:HD3	1.89	0.42
1:A:141:GLN:HE21	1:A:145:ARG:HH21	1.67	0.42
2:B:45:ARG:CG	2:B:81:ARG:HH12	2.32	0.42
1:D:156:ARG:HH11	3:F:5:ARG:HB3	1.84	0.42
1:D:55:GLU:HG2	1:D:59:TYR:CD1	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:GLU:OE2	3:F:1:ARG:HD2	2.19	0.42
1:A:200:THR:C	1:A:201:LEU:HD12	2.39	0.42
2:E:19:LYS:O	2:E:72:PRO:HD2	2.20	0.42
1:D:156:ARG:NH1	3:F:5:ARG:HB3	2.35	0.42
1:D:133:TRP:HB2	1:D:144:LYS:HG3	2.01	0.42
1:A:103:LEU:HD23	1:A:103:LEU:HA	1.80	0.42
1:A:7:TYR:O	1:A:98:MET:HA	2.19	0.42
1:D:159:TYR:CD1	1:D:160:LEU:HD12	2.54	0.42
1:D:238:ASP:OD2	1:D:238:ASP:N	2.53	0.42
1:D:253:GLU:OE2	1:D:256:ARG:HD2	2.20	0.42
1:A:82:ARG:NH2	1:A:87:GLN:O	2.52	0.42
1:D:135:ALA:HB1	1:D:140:ALA:HB3	2.01	0.41
2:E:52:SER:OG	2:E:53:ASP:OD2	2.22	0.41
1:A:63:GLU:O	1:A:67:THR:CG2	2.63	0.41
3:C:9:LEU:N	3:C:9:LEU:CD1	2.83	0.41
1:A:115:GLN:HG3	2:B:60:TRP:CZ2	2.56	0.41
1:A:98:MET:CE	1:A:113:TYR:HE2	2.33	0.41
1:D:45:MET:HG2	1:D:67:THR:HG21	2.01	0.41
2:B:21:ASN:HB3	2:B:70:PHE:CE1	2.56	0.41
1:D:213:ILE:CG2	1:D:263:HIS:CE1	2.94	0.41
1:A:54:GLN:HG3	2:E:20:SER:HB2	2.02	0.41
1:D:262:GLN:HE21	1:D:262:GLN:N	2.18	0.41
1:D:185:PRO:HG3	1:D:263:HIS:CD2	2.56	0.41
1:D:8:PHE:HA	1:D:97:TRP:O	2.21	0.41
2:B:25:CYS:O	2:B:65:LEU:HD12	2.21	0.41
1:D:121:LYS:HZ1	2:E:1:ILE:HD12	1.85	0.41
1:D:244:TRP:HZ3	2:E:99:MET:O	2.03	0.41
2:B:89:GLN:OE1	2:B:91:LYS:HG2	2.21	0.40
1:A:109:LEU:H	1:A:109:LEU:HD23	1.86	0.40
1:D:111:ARG:HD3	1:D:112:GLY:N	2.35	0.40
1:D:117:ALA:HB2	2:E:60:TRP:CE2	2.55	0.40
1:D:234:ARG:HH21	2:E:8:GLN:HE21	1.69	0.40
1:D:24:ALA:O	1:D:25:MET:HG3	2.22	0.40
1:D:272:LEU:HD23	1:D:273:ARG:HH21	1.87	0.40
2:E:39:LEU:O	2:E:46:ILE:HG12	2.21	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	263/276 (95%)	231 (88%)	23 (9%)	9 (3%)	3	24
1	D	256/276 (93%)	229 (90%)	20 (8%)	7 (3%)	5	30
2	B	97/100 (97%)	89 (92%)	7 (7%)	1 (1%)	15	54
2	E	97/100 (97%)	86 (89%)	8 (8%)	3 (3%)	4	26
3	C	7/9 (78%)	6 (86%)	0	1 (14%)	0	1
3	F	7/9 (78%)	7 (100%)	0	0	100	100
All	All	727/770 (94%)	648 (89%)	58 (8%)	21 (3%)	4	28

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	107	GLY
1	D	251	SER
2	E	48	LYS
1	A	219	ARG
1	A	251	SER
2	B	52	SER
1	A	269	PRO
1	D	228	VAL
2	E	53	ASP
1	A	129	ASP
1	A	252	GLY
1	D	86	ASN
1	D	250	PRO
1	A	192	HIS
1	A	221	GLY
3	C	4	PRO
1	D	269	PRO
1	D	192	HIS
1	D	252	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	14	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	225/232 (97%)	183 (81%)	42 (19%)	1	8
1	D	220/232 (95%)	177 (80%)	43 (20%)	1	7
2	B	94/95 (99%)	79 (84%)	15 (16%)	2	11
2	E	94/95 (99%)	78 (83%)	16 (17%)	2	10
3	C	9/9 (100%)	7 (78%)	2 (22%)	1	4
3	F	9/9 (100%)	6 (67%)	3 (33%)	0	0
All	All	651/672 (97%)	530 (81%)	121 (19%)	1	8

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	MET
1	A	44	ARG
1	A	58	GLU
1	A	63	GLU
1	A	67	THR
1	A	72	GLN
1	A	76	MET
1	A	81	LEU
1	A	86	ASN
1	A	94	THR
1	A	96	GLN
1	A	102	ASP
1	A	121	LYS
1	A	124	LEU
1	A	126	LEU
1	A	152	VAL
1	A	154	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	170	ARG
1	A	177	GLU
1	A	192	HIS
1	A	195	PHE
1	A	200	THR
1	A	214	ILE
1	A	216	THR
1	A	218	GLN
1	A	222	GLU
1	A	226	GLN
1	A	230	LEU
1	A	231	VAL
1	A	233	THR
1	A	234	ARG
1	A	244	TRP
1	A	247	VAL
1	A	251	SER
1	A	253	GLU
1	A	254	GLU
1	A	255	GLN
1	A	259	CYS
1	A	260	HIS
1	A	268	GLU
1	A	270	LEU
1	A	271	MET
2	B	12	ARG
2	B	21	ASN
2	B	23	LEU
2	B	39	LEU
2	B	48	LYS
2	B	57	SER
2	B	58	LYS
2	B	64	LEU
2	B	70	PHE
2	B	86	THR
2	B	87	LEU
2	B	88	SER
2	B	89	GLN
2	B	91	LYS
2	B	99	MET
3	C	7	LEU
3	C	9	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	6	ARG
1	D	14	ARG
1	D	19	GLU
1	D	25	MET
1	D	34	VAL
1	D	42	CYS
1	D	58	GLU
1	D	65	ARG
1	D	78	LEU
1	D	81	LEU
1	D	97	TRP
1	D	99	ILE
1	D	101	CYS
1	D	103	LEU
1	D	105	SER
1	D	109	LEU
1	D	111	ARG
1	D	124	LEU
1	D	151	ASN
1	D	156	ARG
1	D	164	CYS
1	D	168	LEU
1	D	170	ARG
1	D	183	ASP
1	D	190	THR
1	D	195	PHE
1	D	203	CYS
1	D	213	ILE
1	D	222	GLU
1	D	223	ASP
1	D	226	GLN
1	D	227	ASP
1	D	231	VAL
1	D	233	THR
1	D	238	ASP
1	D	244	TRP
1	D	247	VAL
1	D	255	GLN
1	D	259	CYS
1	D	261	VAL
1	D	262	GLN
1	D	272	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	273	ARG
2	E	19	LYS
2	E	23	LEU
2	E	26	TYR
2	E	27	VAL
2	E	34	ASP
2	E	38	ASP
2	E	48	LYS
2	E	54	LEU
2	E	71	THR
2	E	74	GLU
2	E	75	LYS
2	E	83	ASN
2	E	88	SER
2	E	89	GLN
2	E	92	ILE
2	E	98	ASP
3	F	1	ARG
3	F	5	ARG
3	F	9	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	32	GLN
1	A	54	GLN
1	A	66	ASN
1	A	72	GLN
1	A	93	HIS
1	A	96	GLN
1	A	127	ASN
1	A	174	ASN
1	A	218	GLN
1	A	226	GLN
2	B	2	GLN
2	B	8	GLN
2	B	17	ASN
2	B	21	ASN
2	B	31	HIS
1	D	32	GLN
1	D	66	ASN

Continued from previous page...

Mol	Chain	Res	Type
1	D	141	GLN
1	D	174	ASN
1	D	242	GLN
1	D	262	GLN
2	E	8	GLN
2	E	24	ASN
2	E	42	ASN
2	E	51	HIS
2	E	83	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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 (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	269/276 (97%)	-0.23	0	100	100	31, 40, 66, 68	0
1	D	262/276 (94%)	-0.10	3 (1%)	80	69	31, 40, 66, 70	0
2	B	99/100 (99%)	-0.32	0	100	100	39, 44, 51, 56	0
2	E	99/100 (99%)	-0.10	1 (1%)	82	72	38, 43, 50, 56	0
3	C	9/9 (100%)	-0.17	0	100	100	38, 41, 45, 45	0
3	F	9/9 (100%)	-0.09	0	100	100	39, 42, 46, 46	0
All	All	747/770 (97%)	-0.18	4 (0%)	91	86	31, 42, 65, 70	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	263	HIS	2.5
1	D	223	ASP	2.4
2	E	10	TYR	2.2
1	D	1	GLY	2.1

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.