



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:35 AM EDT

PDB ID : 6AVG / pdb_00006avg
Title : Crystal structure of the KFJ37 TCR-NY-ESO-1-HLA-B*07:02 complex
Authors : Gully, B.S.; Gras, S.; Rossjohn, J.
Deposited on : 2017-09-02
Resolution : 2.60 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

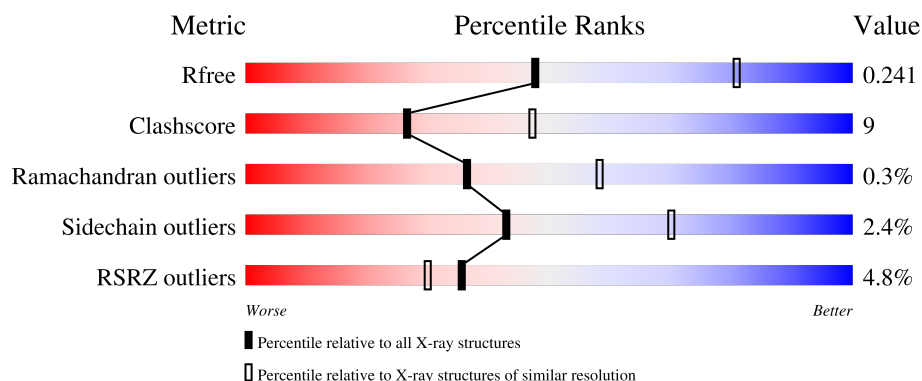
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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.



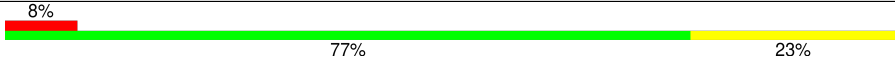
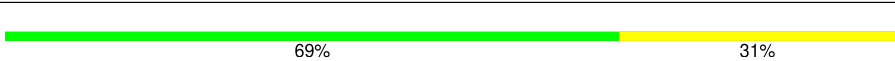
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 $\leq 5\%$. 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	107	6% 74% 18% 7%
1	H	107	77% 15% 7%
2	B	202	6% 76% 20% ..
2	C	202	5% 78% 18% ..
3	D	245	2% 82% 17% .

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Mol	Chain	Length	Quality of chain
3	E	245	
4	F	362	
4	G	362	
5	P	13	
5	Q	13	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13701 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 Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			
1	A	99	Total	C	N	O	S	0	0	0
			829	528	140	158	3			

- Molecule 2 is a protein called T-cell receptor alpha variable 4,TCR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	196	Total	C	N	O	S	0	1	0
			1526	958	251	309	8			
2	B	196	Total	C	N	O	S	0	0	0
			1519	955	248	308	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	3	MET	-	initiating methionine	UNP A0A0B4J268
C	94	VAL	GLY	conflict	UNP A0A0B4J268
B	3	MET	-	initiating methionine	UNP A0A0B4J268
B	94	VAL	GLY	conflict	UNP A0A0B4J268

- Molecule 3 is a protein called T-cell receptor beta variable 9,TCR beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	245	Total	C	N	O	S	0	0	0
			1933	1216	339	372	6			
3	E	245	Total	C	N	O	S	0	0	0
			1927	1213	336	372	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	3	MET	-	initiating methionine	UNP A0A0B4J1U6
D	51	GLN	HIS	conflict	UNP A0A0B4J1U6
D	98	GLY	VAL	conflict	UNP A0A0B4J1U6
E	3	MET	-	initiating methionine	UNP A0A0B4J1U6
E	51	GLN	HIS	conflict	UNP A0A0B4J1U6
E	98	GLY	VAL	conflict	UNP A0A0B4J1U6

- Molecule 4 is a protein called HLA class I histocompatibility antigen, B-7 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	272	Total	C	N	O	S	8	0	0
			2221	1381	408	426	6			
4	F	275	Total	C	N	O	S	0	0	0
			2251	1397	413	435	6			

- Molecule 5 is a protein called ALA-PRO-ARG-GLY-PRO-HIS-GLY-GLY-ALA-ALA-SER-GLY-LEU.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	Q	13	Total	C	N	O	0	0	0
			81	48	18	15			
5	P	13	Total	C	N	O	0	0	0
			81	48	18	15			

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	36	Total	O	0	0
			36	36		
6	C	65	Total	O	0	0
			65	65		
6	D	47	Total	O	0	0
			47	47		
6	G	85	Total	O	0	0
			85	85		
6	A	42	Total	O	0	0
			42	42		
6	B	80	Total	O	0	0
			80	80		
6	E	43	Total	O	0	0
			43	43		
6	F	93	Total	O	0	0
			93	93		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	Q	7	Total	O	0	0
			7	7		
6	P	6	Total	O	0	0
			6	6		

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: Beta-2-microglobulin

Chain H: 



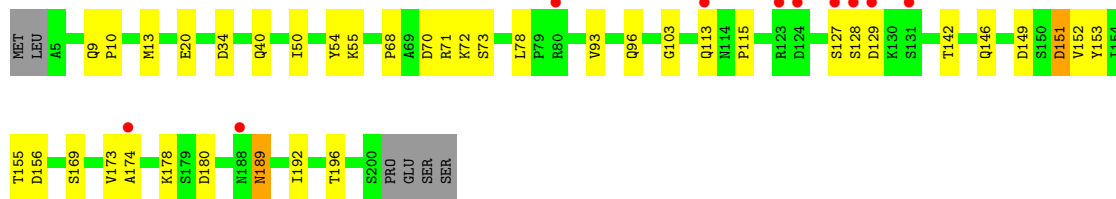
- Molecule 1: Beta-2-microglobulin

Chain A: 



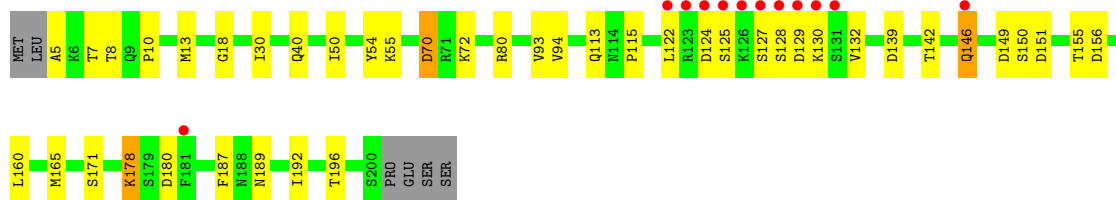
- Molecule 2: T-cell receptor alpha variable 4,TCR alpha chain

Chain C: 

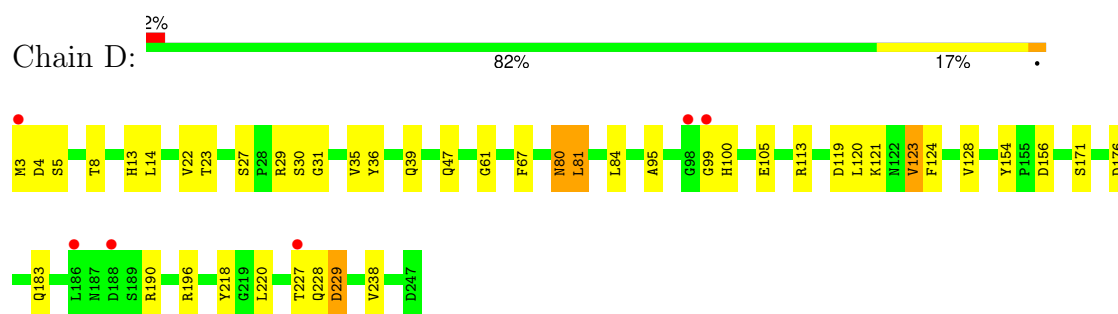


- Molecule 2: T-cell receptor alpha variable 4,TCR alpha chain

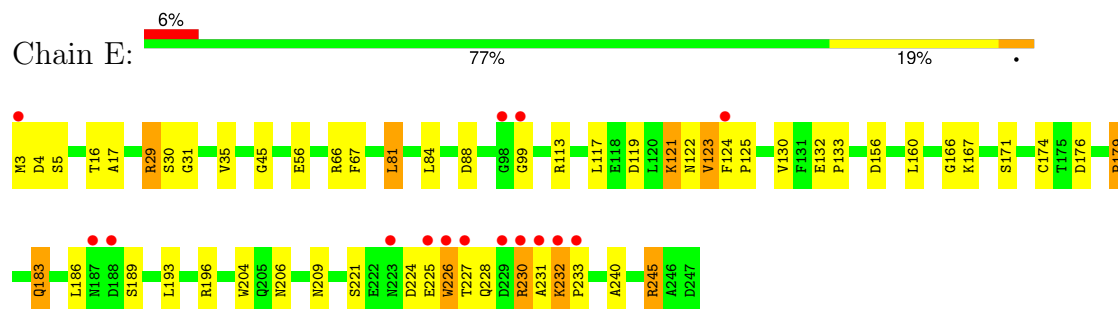
Chain B: 



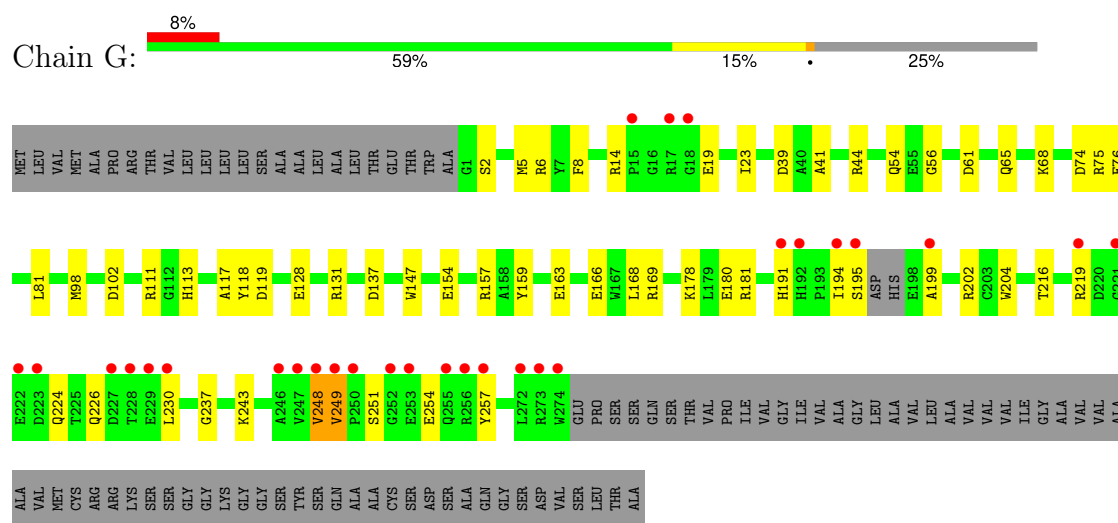
- Molecule 3: T-cell receptor beta variable 9,TCR beta chain



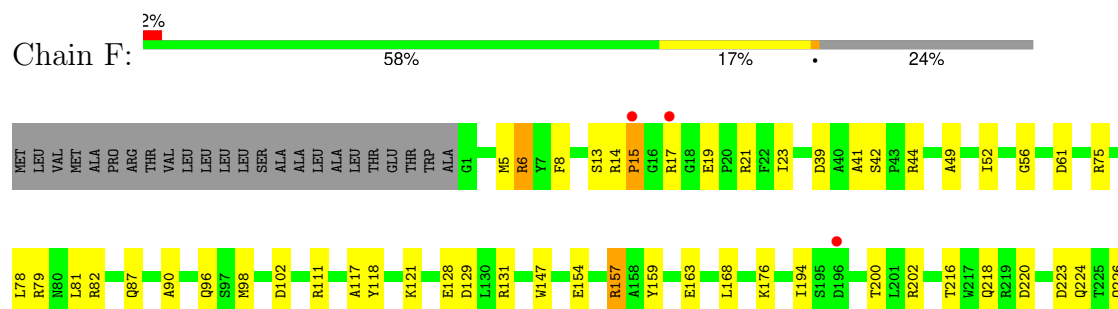
- Molecule 3: T-cell receptor beta variable 9,TCR beta chain

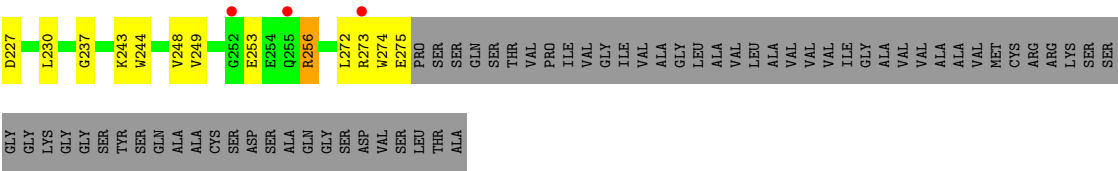


- Molecule 4: HLA class I histocompatibility antigen, B-7 alpha chain



- Molecule 4: HLA class I histocompatibility antigen, B-7 alpha chain

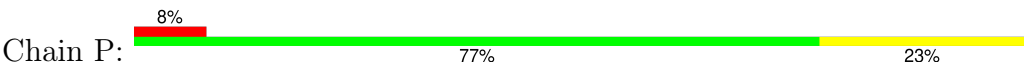




● Molecule 5: ALA-PRO-ARG-GLY-PRO-HIS-GLY-GLY-ALA-ALA-SER-GLY-LEU



● Molecule 5: ALA-PRO-ARG-GLY-PRO-HIS-GLY-GLY-ALA-ALA-SER-GLY-LEU



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.81Å 74.86Å 96.28Å 94.22° 97.88° 90.16°	Depositor
Resolution (Å)	38.81 – 2.60 38.81 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (38.81-2.60) 98.8 (38.81-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.193 , 0.248 0.194 , 0.241	Depositor DCC
R_{free} test set	2842 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13701	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.30	0/852	0.67	0/1152
1	H	0.30	0/852	0.70	0/1152
2	B	0.33	0/1552	0.89	4/2117 (0.2%)
2	C	0.33	0/1559	0.84	4/2127 (0.2%)
3	D	0.33	0/1984	0.83	3/2699 (0.1%)
3	E	0.43	1/1978 (0.1%)	0.85	5/2692 (0.2%)
4	F	0.34	0/2313	0.81	5/3142 (0.2%)
4	G	0.38	0/2281	0.92	5/3097 (0.2%)
5	P	0.41	0/83	1.32	0/110
5	Q	0.38	0/83	1.32	0/110
All	All	0.35	1/13537 (0.0%)	0.84	26/18398 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	231	ALA	CA-CB	-5.84	1.44	1.53

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	249	VAL	CA-C-N	-13.74	106.01	120.85
4	G	249	VAL	C-N-CA	-13.74	106.01	120.85
3	E	232	LYS	N-CA-C	9.66	124.21	110.40
2	B	189	ASN	N-CA-C	-7.11	104.09	114.39
3	E	226	TRP	CA-CB-CG	-6.84	100.60	113.60
2	C	78	LEU	CA-C-N	6.38	125.60	118.97
2	C	78	LEU	C-N-CA	6.38	125.60	118.97
2	C	151	ASP	N-CA-C	-6.21	105.70	113.28
2	B	187	PHE	N-CA-C	6.17	120.12	112.59
4	F	224	GLN	CA-CB-CG	6.05	126.20	114.10
4	F	224	GLN	N-CA-CB	6.05	117.13	110.35
4	G	56	GLY	CA-C-N	5.76	125.89	119.32
4	G	56	GLY	C-N-CA	5.76	125.89	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	225	GLU	CA-C-N	-5.73	115.14	122.77
3	E	225	GLU	C-N-CA	-5.73	115.14	122.77
3	D	176	ASP	CA-C-N	5.73	127.00	119.84
3	D	176	ASP	C-N-CA	5.73	127.00	119.84
2	B	178	LYS	N-CA-C	5.54	118.06	110.24
3	D	227	THR	N-CA-C	5.43	120.06	113.38
4	F	256	ARG	N-CA-C	-5.40	105.50	113.61
4	F	56	GLY	CA-C-N	5.37	125.44	119.32
4	F	56	GLY	C-N-CA	5.37	125.44	119.32
2	C	189	ASN	N-CA-C	-5.34	106.65	114.39
3	E	179	PRO	N-CA-C	5.25	118.84	111.33
4	G	180	GLU	N-CA-C	-5.17	107.14	112.93
2	B	94	VAL	N-CA-C	5.04	115.38	108.12

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	829	0	794	16	0
1	H	829	0	794	11	0
2	B	1519	0	1433	28	0
2	C	1526	0	1434	26	0
3	D	1933	0	1826	33	0
3	E	1927	0	1815	41	0
4	F	2251	0	2094	44	0
4	G	2221	0	2074	49	0
5	P	81	0	79	3	0
5	Q	81	0	79	4	0
6	A	42	0	0	4	1
6	B	80	0	0	5	1
6	C	65	0	0	7	0
6	D	47	0	0	5	0
6	E	43	0	0	7	0
6	F	93	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	85	0	0	11	0
6	H	36	0	0	1	0
6	P	6	0	0	0	0
6	Q	7	0	0	1	0
All	All	13701	0	12422	238	1

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 9.

All (238) 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)
4:G:191:HIS:HE1	4:G:199:ALA:HB1	1.26	1.00
1:A:1:ILE:HD11	4:F:121:LYS:HZ2	1.27	0.98
3:D:80:ASN:N	3:D:80:ASN:HD22	1.63	0.95
3:E:179:PRO:O	6:E:301:HOH:O	1.84	0.93
1:A:1:ILE:HD11	4:F:121:LYS:NZ	1.88	0.87
2:B:149:ASP:HB3	2:B:151:ASP:OD1	1.75	0.86
4:G:169:ARG:NH1	6:G:404:HOH:O	2.09	0.86
2:C:9:GLN:OE1	6:C:301:HOH:O	1.93	0.85
4:G:199:ALA:N	4:G:249:VAL:O	2.10	0.84
4:G:44:ARG:NH2	4:G:61:ASP:OD1	2.10	0.83
3:E:3:MET:HB3	3:E:4:ASP:HA	1.61	0.82
3:D:23:THR:HG22	3:D:80:ASN:HB3	1.61	0.82
2:C:20:GLU:OE2	6:C:302:HOH:O	1.98	0.80
3:D:171:SER:OG	6:D:301:HOH:O	2.00	0.80
3:E:125:PRO:HD3	3:E:233:PRO:HB3	1.64	0.78
3:D:80:ASN:HD22	3:D:80:ASN:H	1.31	0.78
4:F:14:ARG:HB3	4:F:17:ARG:HB2	1.64	0.78
3:D:113:ARG:NH1	3:D:156:ASP:O	2.17	0.77
4:G:191:HIS:CE1	4:G:199:ALA:HB1	2.16	0.77
3:D:3:MET:HB3	3:D:4:ASP:HA	1.66	0.77
4:F:6:ARG:NH2	4:F:102:ASP:OD1	2.17	0.76
4:G:131:ARG:O	6:G:402:HOH:O	2.03	0.75
4:F:41:ALA:O	6:F:402:HOH:O	2.04	0.75
4:G:44:ARG:O	6:G:403:HOH:O	2.05	0.73
2:C:103:GLY:O	6:C:303:HOH:O	2.06	0.73
1:A:50:GLU:OE1	6:A:101:HOH:O	2.08	0.72
3:E:3:MET:SD	6:E:337:HOH:O	2.47	0.71
2:C:54:TYR:O	2:C:71:ARG:NH1	2.23	0.70
2:C:155:THR:HG21	3:D:196:ARG:HH12	1.56	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:THR:O	6:B:301:HOH:O	2.09	0.69
2:B:40:GLN:HB2	2:B:50:ILE:HD11	1.75	0.69
4:F:176:LYS:NZ	6:F:405:HOH:O	2.25	0.69
2:B:30:ILE:O	6:B:302:HOH:O	2.11	0.68
2:B:70:ASP:HB3	2:B:72:LYS:HG3	1.74	0.68
4:G:74:ASP:OD2	6:G:406:HOH:O	2.11	0.68
2:C:129:ASP:O	6:C:304:HOH:O	2.11	0.67
2:B:10:PRO:HG2	2:B:13:MET:HE3	1.77	0.67
2:C:113:GLN:C	2:C:115:PRO:HD3	2.19	0.67
3:E:160:LEU:O	6:E:302:HOH:O	2.12	0.67
2:C:40:GLN:HB2	2:C:50:ILE:HD11	1.78	0.66
2:B:5:ALA:O	6:B:303:HOH:O	2.12	0.66
3:E:119:ASP:OD2	3:E:121:LYS:HG3	1.96	0.66
4:F:8:PHE:HE2	4:F:98:MET:HE3	1.59	0.65
4:G:2:SER:OG	6:G:405:HOH:O	2.09	0.65
3:D:81:LEU:HB3	3:D:84:LEU:HD21	1.78	0.64
3:D:39:GLN:OE1	6:D:302:HOH:O	2.15	0.64
3:D:3:MET:N	3:D:29:ARG:HE	1.94	0.64
1:H:54:LEU:HB3	4:G:23:ILE:HD13	1.79	0.64
4:F:79:ARG:NH2	6:F:407:HOH:O	2.31	0.64
4:G:219:ARG:HB2	4:G:224:GLN:HE21	1.63	0.63
2:C:10:PRO:HG2	2:C:13:MET:HE3	1.80	0.63
4:G:8:PHE:HE2	4:G:98:MET:HE3	1.64	0.62
3:E:81:LEU:HB3	3:E:84:LEU:HD21	1.79	0.62
4:F:44:ARG:NH2	4:F:61:ASP:OD1	2.29	0.62
4:G:111:ARG:NH2	4:G:128:GLU:OE2	2.33	0.61
2:C:70:ASP:HB2	2:C:72:LYS:HG3	1.83	0.60
3:E:3:MET:HB3	3:E:4:ASP:CA	2.31	0.60
4:F:96:GLN:OE1	6:F:403:HOH:O	2.16	0.60
4:F:131:ARG:HH12	4:F:157:ARG:NH2	1.99	0.60
4:F:147:TRP:HE1	5:Q:11:SER:HB2	1.66	0.60
3:E:166:GLY:C	3:E:167:LYS:HD3	2.27	0.59
3:E:183:GLN:O	3:E:189:SER:OG	2.11	0.59
4:F:220:ASP:OD2	4:F:256:ARG:NH2	2.31	0.59
4:F:200:THR:HG22	4:F:248:VAL:HG22	1.84	0.59
4:G:5:MET:HB2	4:G:168:LEU:HD13	1.84	0.59
2:C:149:ASP:HB3	2:C:151:ASP:OD1	2.03	0.59
3:D:80:ASN:N	3:D:80:ASN:ND2	2.37	0.59
3:E:226:TRP:HE1	3:E:228:GLN:HA	1.68	0.59
4:G:137:ASP:OD1	6:G:407:HOH:O	2.17	0.58
2:C:155:THR:HG21	3:D:196:ARG:NH1	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:G:254:GLU:HA	4:G:257:TYR:CD2	2.38	0.58
4:G:131:ARG:HH12	4:G:157:ARG:NH2	2.02	0.57
4:G:230:LEU:HD11	4:G:243:LYS:HE3	1.85	0.57
4:G:54:GLN:NE2	6:G:414:HOH:O	2.31	0.57
3:E:56:GLU:OE2	4:F:75:ARG:NH2	2.37	0.56
3:E:171:SER:OG	6:E:303:HOH:O	2.18	0.56
3:E:226:TRP:NE1	3:E:228:GLN:HA	2.20	0.56
4:F:194:ILE:HD11	4:F:200:THR:HG23	1.87	0.56
4:G:219:ARG:HB2	4:G:224:GLN:NE2	2.21	0.56
2:B:192:ILE:HD11	2:B:196:THR:HG21	1.87	0.56
5:P:12:GLY:O	5:P:13:LEU:HB2	2.07	0.55
4:G:65:GLN:NE2	6:G:423:HOH:O	2.39	0.55
4:G:14:ARG:NH2	4:G:39:ASP:OD2	2.36	0.55
3:E:226:TRP:NE1	3:E:227:THR:O	2.40	0.55
2:C:34:ASP:O	2:C:71:ARG:NH2	2.36	0.54
3:D:120:LEU:HD13	3:D:220:LEU:HD22	1.89	0.54
1:H:24:ASN:HB3	1:H:65:LEU:HD11	1.89	0.54
4:G:147:TRP:HE1	5:P:11:SER:HB2	1.73	0.54
5:Q:3:ARG:NH1	6:Q:101:HOH:O	2.20	0.54
2:B:171:SER:HB3	6:B:324:HOH:O	2.08	0.53
2:B:54:TYR:CD2	2:B:55:LYS:HG3	2.43	0.53
2:C:54:TYR:CD2	2:C:55:LYS:HG3	2.44	0.53
3:D:61:GLY:O	6:D:303:HOH:O	2.19	0.53
4:G:111:ARG:HE	4:G:113:HIS:CE1	2.26	0.53
3:D:5:SER:OG	3:D:30:SER:OG	2.25	0.53
1:H:60:TRP:CE2	4:G:117:ALA:HB2	2.43	0.53
4:F:13:SER:HB3	4:F:78:LEU:HD13	1.91	0.53
3:E:226:TRP:CD1	3:E:232:LYS:HG3	2.45	0.52
4:F:82:ARG:NH1	4:F:87:GLN:O	2.36	0.52
2:B:5:ALA:HB3	2:B:93:VAL:HG21	1.91	0.52
3:E:226:TRP:CZ2	3:E:232:LYS:HD2	2.46	0.51
1:A:96:ASP:HB3	1:A:99:MET:HG3	1.90	0.51
1:A:23:LEU:O	1:A:67:TYR:HA	2.11	0.51
2:B:146:GLN:CD	2:B:146:GLN:H	2.19	0.51
1:A:24:ASN:HB3	1:A:65:LEU:HD11	1.92	0.51
3:D:228:GLN:HG2	3:D:229:ASP:N	2.25	0.50
2:B:18:GLY:O	2:B:80:ARG:NH1	2.45	0.50
4:F:111:ARG:NH2	4:F:128:GLU:OE2	2.44	0.50
3:D:80:ASN:H	3:D:80:ASN:ND2	2.02	0.50
4:G:254:GLU:HA	4:G:257:TYR:CE2	2.47	0.50
4:F:253:GLU:HB2	4:F:256:ARG:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3:MET:HB3	3:D:4:ASP:CA	2.38	0.50
3:E:228:GLN:NE2	3:E:230:ARG:O	2.44	0.50
4:F:5:MET:HB2	4:F:168:LEU:HD13	1.93	0.50
1:H:23:LEU:O	1:H:67:TYR:HA	2.12	0.49
4:G:6:ARG:NH1	4:G:102:ASP:OD1	2.43	0.49
4:G:202:ARG:HG2	4:G:204:TRP:NE1	2.28	0.49
3:E:221:SER:N	3:E:224:ASP:OD2	2.41	0.49
5:Q:12:GLY:O	5:Q:13:LEU:HB2	2.13	0.49
2:C:155:THR:HB	2:C:173:VAL:H	1.78	0.49
1:H:58:LYS:HA	4:G:98:MET:HE1	1.95	0.49
3:E:132:GLU:OE1	3:E:245:ARG:NH1	2.46	0.48
2:B:155:THR:HG21	3:E:196:ARG:HH12	1.77	0.48
2:C:96:GLN:NE2	6:C:306:HOH:O	2.25	0.48
6:A:103:HOH:O	4:F:237:GLY:HA3	2.13	0.48
2:C:192:ILE:HD11	2:C:196:THR:HG21	1.95	0.48
4:G:61:ASP:O	4:G:65:GLN:HG2	2.14	0.48
4:F:147:TRP:NE1	5:Q:11:SER:HB2	2.28	0.47
4:F:21:ARG:HH21	4:F:23:ILE:HD11	1.79	0.47
3:E:122:ASN:OD1	3:E:122:ASN:N	2.46	0.47
1:H:96:ASP:OD2	1:H:99:MET:HE3	2.15	0.47
3:D:124:PHE:CD1	3:D:190:ARG:HD3	2.50	0.47
4:F:15:PRO:HB3	4:F:90:ALA:O	2.14	0.47
3:D:119:ASP:OD2	3:D:121:LYS:HG3	2.15	0.47
4:F:230:LEU:HD11	4:F:243:LYS:HE3	1.96	0.47
2:C:169:SER:HA	6:C:314:HOH:O	2.15	0.47
4:F:14:ARG:NH2	4:F:21:ARG:HB2	2.29	0.47
4:F:19:GLU:HG3	4:F:75:ARG:NH2	2.30	0.47
3:E:5:SER:OG	3:E:30:SER:OG	2.30	0.47
4:F:14:ARG:NH2	4:F:39:ASP:OD2	2.44	0.47
4:F:42:SER:HA	6:F:402:HOH:O	2.15	0.46
2:B:150:SER:O	2:B:150:SER:OG	2.33	0.46
2:B:155:THR:HG22	2:B:156:ASP:O	2.15	0.46
2:B:113:GLN:C	2:B:115:PRO:HD3	2.40	0.46
2:B:165:MET:HE2	2:B:165:MET:HB3	1.86	0.46
2:B:130:LYS:H	2:B:130:LYS:HD2	1.80	0.46
3:E:113:ARG:NH2	6:E:314:HOH:O	2.48	0.46
4:F:274:TRP:HA	4:F:275:GLU:HA	1.70	0.46
4:G:131:ARG:HH12	4:G:157:ARG:CZ	2.28	0.46
3:D:47:GLN:OE1	6:D:302:HOH:O	2.21	0.46
1:H:1:ILE:HG13	4:G:119:ASP:O	2.16	0.45
3:D:31:GLY:O	3:D:99:GLY:HA3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:113:ARG:NH1	3:E:156:ASP:O	2.50	0.45
4:F:8:PHE:CE2	4:F:98:MET:HE3	2.45	0.45
1:A:60:TRP:CE2	4:F:117:ALA:HB2	2.51	0.45
3:D:105:GLU:OE1	6:D:304:HOH:O	2.21	0.45
3:D:128:VAL:HG21	3:D:238:VAL:O	2.16	0.45
3:D:67:PHE:CE1	3:D:81:LEU:HG	2.52	0.45
4:G:81:LEU:HD13	4:G:118:TYR:CD1	2.52	0.45
2:B:178:LYS:HD3	2:B:180:ASP:HB3	1.99	0.45
3:E:166:GLY:O	3:E:167:LYS:HD3	2.17	0.45
3:E:130:VAL:HG23	3:E:240:ALA:HB3	1.99	0.45
3:D:22:VAL:HG22	3:D:84:LEU:HD11	1.99	0.44
3:D:119:ASP:CG	3:D:121:LYS:HG3	2.43	0.44
4:G:219:ARG:HD3	4:G:219:ARG:C	2.42	0.44
1:H:73:THR:HG22	1:H:75:LYS:H	1.81	0.44
2:C:153:TYR:O	2:C:174:ALA:HA	2.17	0.44
1:A:96:ASP:OD2	1:A:99:MET:HE3	2.17	0.44
2:B:124:ASP:OD1	2:B:124:ASP:C	2.61	0.44
3:E:17:ALA:HA	3:E:117:LEU:O	2.16	0.44
3:E:176:ASP:HB2	3:E:193:LEU:HD12	2.00	0.44
1:A:46:ILE:O	6:A:102:HOH:O	2.21	0.44
4:F:87:GLN:NE2	6:F:417:HOH:O	2.48	0.44
4:G:19:GLU:CD	4:G:75:ARG:HH11	2.26	0.44
4:F:81:LEU:HD13	4:F:118:TYR:CD1	2.53	0.44
4:F:218:GLN:HG2	4:F:223:ASP:HA	2.00	0.44
2:B:70:ASP:N	2:B:70:ASP:OD1	2.51	0.44
3:E:31:GLY:O	3:E:99:GLY:HA3	2.18	0.44
3:E:206:ASN:HB3	3:E:209:ASN:ND2	2.32	0.44
1:A:1:ILE:HD12	1:A:1:ILE:O	2.18	0.44
4:F:202:ARG:HD2	4:F:244:TRP:CD2	2.53	0.44
3:D:13:HIS:CD2	3:D:218:TYR:HB3	2.53	0.43
4:G:76:GLU:HB3	6:G:420:HOH:O	2.19	0.43
2:B:124:ASP:HA	2:B:125:SER:HA	1.76	0.43
4:G:68:LYS:O	6:G:408:HOH:O	2.21	0.43
4:G:178:LYS:O	4:G:181:ARG:HB3	2.19	0.43
1:A:23:LEU:HB3	1:A:68:THR:HG22	2.01	0.43
3:E:45:GLY:O	6:E:304:HOH:O	2.21	0.43
2:C:151:ASP:OD1	2:C:152:VAL:HG23	2.18	0.43
4:F:159:TYR:HA	4:F:163:GLU:OE1	2.19	0.43
2:C:155:THR:HG22	2:C:156:ASP:O	2.19	0.43
3:E:122:ASN:HA	3:E:124:PHE:CE2	2.54	0.43
3:E:3:MET:HG3	3:E:29:ARG:NH1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:ILE:HA	1:A:2:GLN:HG3	2.01	0.42
3:E:66:ARG:NH1	3:E:88:ASP:OD2	2.39	0.42
3:E:123:VAL:O	3:E:233:PRO:HG3	2.19	0.42
4:F:226:GLN:O	4:F:227:ASP:HB2	2.19	0.42
2:C:68:PRO:HD2	2:C:73:SER:O	2.19	0.42
3:D:36:TYR:HB2	3:D:95:ALA:HB3	2.00	0.42
2:B:8:THR:HA	6:B:349:HOH:O	2.19	0.42
2:B:139:ASP:C	2:B:139:ASP:OD1	2.62	0.42
1:H:1:ILE:HA	1:H:2:GLN:HG3	2.00	0.42
4:G:199:ALA:O	4:G:249:VAL:N	2.44	0.42
4:G:254:GLU:HA	4:G:257:TYR:HD2	1.83	0.42
2:B:127:SER:HA	2:B:128:SER:HA	1.79	0.42
3:E:67:PHE:CE1	3:E:81:LEU:HG	2.54	0.42
3:E:226:TRP:CD1	3:E:228:GLN:HA	2.55	0.42
4:F:129:ASP:O	4:F:131:ARG:HG3	2.19	0.42
2:C:146:GLN:O	2:C:189:ASN:ND2	2.50	0.42
4:G:147:TRP:NE1	5:P:11:SER:HB2	2.33	0.42
6:C:361:HOH:O	4:G:166:GLU:HG2	2.19	0.42
1:H:23:LEU:HB2	1:H:70:PHE:CE2	2.55	0.42
4:G:199:ALA:O	4:G:248:VAL:HA	2.20	0.42
3:E:167:LYS:NZ	6:E:308:HOH:O	2.37	0.42
3:D:123:VAL:HG23	3:D:154:TYR:O	2.20	0.41
1:A:19:LYS:O	1:A:72:PRO:HD2	2.20	0.41
2:B:160:LEU:HB3	3:E:174:CYS:HB2	2.02	0.41
1:A:94:LYS:NZ	6:A:109:HOH:O	2.52	0.41
4:G:249:VAL:HG11	4:G:257:TYR:CE1	2.56	0.41
3:E:133:PRO:HD2	3:E:204:TRP:CZ2	2.55	0.41
3:D:8:THR:OG1	3:D:27:SER:HB2	2.20	0.41
1:H:19:LYS:O	1:H:72:PRO:HD2	2.20	0.41
4:G:159:TYR:HA	4:G:163:GLU:OE1	2.21	0.41
2:C:127:SER:HA	2:C:128:SER:HA	1.92	0.41
4:G:41:ALA:HB3	6:G:448:HOH:O	2.20	0.41
2:C:178:LYS:HE3	2:C:180:ASP:HB3	2.02	0.41
4:G:194:ILE:H	4:G:195:SER:HA	1.86	0.41
6:H:105:HOH:O	4:G:237:GLY:HA3	2.20	0.41
3:D:14:LEU:HD12	3:D:14:LEU:HA	1.88	0.41
4:G:131:ARG:NH1	4:G:157:ARG:NH2	2.69	0.40
4:F:14:ARG:HD3	4:F:17:ARG:O	2.20	0.40
4:F:131:ARG:NH1	4:F:157:ARG:NH2	2.69	0.40
1:A:58:LYS:HA	4:F:98:MET:HE1	2.02	0.40
2:B:122:LEU:HD13	2:B:132:VAL:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:34:ASP:HB3	2:C:93:VAL:HB	2.04	0.40
3:D:30:SER:O	3:D:100:HIS:ND1	2.54	0.40
1:A:73:THR:HG22	1:A:75:LYS:H	1.86	0.40
4:F:49:ALA:O	4:F:52:ILE:HG22	2.21	0.40

All (1) 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)
6:A:118:HOH:O	6:B:326:HOH:O[1_565]	2.13	0.07

5.3 Torsion angles

5.3.1 Protein backbone

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	97/107 (91%)	95 (98%)	2 (2%)	0	100	100
1	H	97/107 (91%)	95 (98%)	2 (2%)	0	100	100
2	B	194/202 (96%)	182 (94%)	12 (6%)	0	100	100
2	C	195/202 (96%)	181 (93%)	14 (7%)	0	100	100
3	D	243/245 (99%)	234 (96%)	8 (3%)	1 (0%)	30	51
3	E	243/245 (99%)	231 (95%)	11 (4%)	1 (0%)	30	51
4	F	273/362 (75%)	264 (97%)	8 (3%)	1 (0%)	30	51
4	G	268/362 (74%)	258 (96%)	8 (3%)	2 (1%)	18	38
5	P	11/13 (85%)	10 (91%)	1 (9%)	0	100	100
5	Q	11/13 (85%)	10 (91%)	1 (9%)	0	100	100
All	All	1632/1858 (88%)	1560 (96%)	67 (4%)	5 (0%)	36	58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	229	ASP
4	G	226	GLN
4	G	251	SER
3	E	230	ARG
4	F	15	PRO

5.3.2 Protein sidechains ⓘ

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	94/100 (94%)	91 (97%)	3 (3%)	34	62
1	H	94/100 (94%)	92 (98%)	2 (2%)	47	73
2	B	174/186 (94%)	170 (98%)	4 (2%)	44	71
2	C	174/186 (94%)	173 (99%)	1 (1%)	78	91
3	D	209/212 (99%)	204 (98%)	5 (2%)	43	70
3	E	208/212 (98%)	199 (96%)	9 (4%)	26	51
4	F	232/297 (78%)	225 (97%)	7 (3%)	36	64
4	G	228/297 (77%)	225 (99%)	3 (1%)	61	82
5	P	6/6 (100%)	6 (100%)	0	100	100
5	Q	6/6 (100%)	6 (100%)	0	100	100
All	All	1425/1602 (89%)	1391 (98%)	34 (2%)	43	70

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

Mol	Chain	Res	Type
1	H	1	ILE
1	H	9	VAL
2	C	142	THR
3	D	35	VAL
3	D	80	ASN
3	D	81	LEU
3	D	123	VAL
3	D	183	GLN
4	G	154	GLU

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Mol	Chain	Res	Type
4	G	216	THR
4	G	248	VAL
1	A	1	ILE
1	A	9	VAL
1	A	74	GLU
2	B	70	ASP
2	B	129	ASP
2	B	142	THR
2	B	146	GLN
3	E	16	THR
3	E	29	ARG
3	E	35	VAL
3	E	81	LEU
3	E	121	LYS
3	E	123	VAL
3	E	183	GLN
3	E	186	LEU
3	E	245	ARG
4	F	6	ARG
4	F	154	GLU
4	F	157	ARG
4	F	216	THR
4	F	249	VAL
4	F	272	LEU
4	F	273	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	80	ASN
3	D	170	HIS
4	G	70	GLN
4	G	115	GLN
4	G	144	GLN
4	G	224	GLN
4	G	255	GLN
1	A	13	HIS
3	E	183	GLN

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 oligosaccharides 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

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, 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	99/107 (92%)	-0.42	1 (1%) 79 76	16, 25, 50, 66	0
1	H	99/107 (92%)	-0.35	0 100 100	20, 28, 51, 65	0
2	B	196/202 (97%)	0.11	12 (6%) 27 22	15, 32, 92, 125	0
2	C	196/202 (97%)	0.11	10 (5%) 33 28	16, 32, 80, 115	1 (0%)
3	D	245/245 (100%)	0.18	6 (2%) 59 54	17, 43, 73, 90	0
3	E	245/245 (100%)	0.37	15 (6%) 27 22	17, 46, 86, 125	0
4	F	275/362 (75%)	-0.15	6 (2%) 62 57	16, 28, 65, 92	0
4	G	272/362 (75%)	0.12	29 (10%) 11 9	17, 29, 103, 124	2 (0%)
5	P	13/13 (100%)	0.10	1 (7%) 19 15	17, 21, 34, 38	0
5	Q	13/13 (100%)	-0.08	0 100 100	14, 20, 35, 35	0
All	All	1653/1858 (88%)	0.06	80 (4%) 35 30	14, 35, 82, 125	3 (0%)

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	127	SER	6.0
2	B	125	SER	5.7
2	B	126	LYS	5.5
4	G	18	GLY	5.1
3	E	231	ALA	4.5
2	B	129	ASP	4.5
3	E	226	TRP	4.4
2	B	123	ARG	4.1
4	G	199	ALA	3.9
4	G	248	VAL	3.8
2	C	128	SER	3.8
4	G	257	TYR	3.8
3	D	3	MET	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	128	SER	3.7
3	E	229	ASP	3.7
3	D	99	GLY	3.6
4	G	274	TRP	3.6
4	G	252	GLY	3.4
2	B	131	SER	3.3
4	G	249	VAL	3.3
2	B	124	ASP	3.3
3	E	230	ARG	3.2
4	G	17	ARG	3.2
3	E	233	PRO	3.1
3	E	98	GLY	3.1
4	G	250	PRO	3.0
2	C	80[A]	ARG	3.0
3	E	225	GLU	2.9
2	C	124	ASP	2.9
4	G	247	VAL	2.9
4	G	195	SER	2.9
2	C	113	GLN	2.9
4	F	255	GLN	2.8
3	E	99	GLY	2.8
4	F	15	PRO	2.8
2	B	146	GLN	2.8
3	E	232	LYS	2.8
5	P	11	SER	2.7
2	C	127	SER	2.7
2	B	130	LYS	2.7
3	E	188	ASP	2.7
4	G	194	ILE	2.6
4	F	273	ARG	2.6
4	G	253	GLU	2.6
4	G	255	GLN	2.6
4	G	223	ASP	2.5
4	F	252	GLY	2.5
2	C	174	ALA	2.5
3	E	3	MET	2.5
4	G	230	LEU	2.5
4	G	222	GLU	2.5
4	G	191	HIS	2.4
3	D	98	GLY	2.4
3	E	227	THR	2.3
2	B	122	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
3	D	227	THR	2.3
2	C	123	ARG	2.3
2	C	188	ASN	2.3
3	E	187	ASN	2.3
2	C	129	ASP	2.3
4	G	219	ARG	2.3
4	G	228	THR	2.2
2	C	131	SER	2.2
3	E	124	PHE	2.2
4	G	256	ARG	2.2
3	D	188	ASP	2.2
4	G	227	ASP	2.2
4	F	196	ASP	2.2
4	G	15	PRO	2.1
3	D	186	LEU	2.1
4	G	221	GLY	2.1
4	G	273	ARG	2.1
4	G	229	GLU	2.1
4	G	272	LEU	2.1
1	A	99	MET	2.1
4	G	192	HIS	2.1
2	B	181	PHE	2.1
4	G	246	ALA	2.0
3	E	223	ASN	2.0
4	F	17	ARG	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 oligosaccharides 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.