



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:31 AM UTC

PDB ID : 2AQ1 / pdb_00002aq1
Title : Crystal structure of T-cell receptor V beta domain variant complexed with superantigen SEC3 mutant
Authors : Cho, S.; Swaminathan, C.P.; Yang, J.; Kerzic, M.C.; Guan, R.; Kieke, M.C.; Kranz, D.M.; Mariuzza, R.A.; Sundberg, E.J.
Deposited on : 2005-08-17
Resolution : 2.10 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:

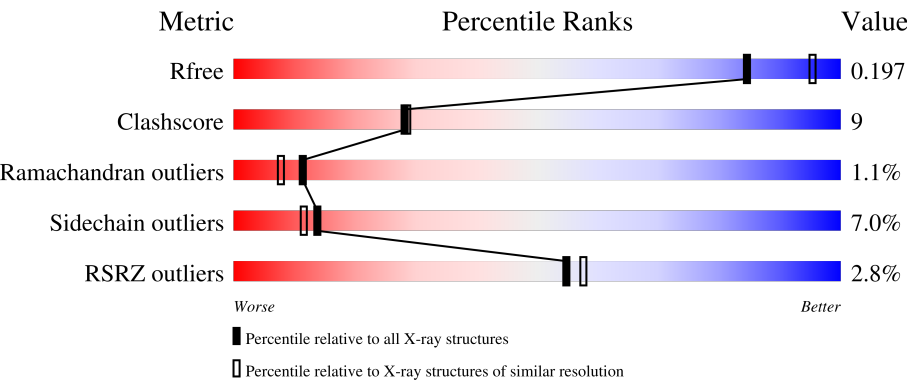
MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	112	3% 87% 8% . .
1	C	112	2% 75% 17% . . .
1	E	112	2% 76% 15% 5% . .
1	G	112	2% 71% 22% . .
2	B	237	% 78% 16% 5% .

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Mol	Chain	Length	Quality of chain
2	D	237	4% 72% 20% 6%
2	F	237	3% 78% 18%
2	H	237	5% 75% 18% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11673 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 T-cell receptor beta chain V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	109	Total	C	N	O	S	0	0	0
			832	517	147	165	3			
1	C	109	Total	C	N	O	S	0	0	0
			832	517	147	165	3			
1	E	109	Total	C	N	O	S	0	0	0
			832	517	147	165	3			
1	G	109	Total	C	N	O	S	0	0	0
			832	517	147	165	3			

- Molecule 2 is a protein called Enterotoxin type C-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	234	Total	C	N	O	S	0	0	0
			1926	1225	316	375	10			
2	D	236	Total	C	N	O	S	0	0	0
			1939	1231	319	379	10			
2	F	237	Total	C	N	O	S	0	0	0
			1948	1236	320	382	10			
2	H	237	Total	C	N	O	S	0	0	0
			1948	1236	320	382	10			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	GLY	SEE REMARK 999	UNP P0A0L5
B	?	-	LYS	SEE REMARK 999	UNP P0A0L5
B	102	TRP	VAL	SEE REMARK 999	UNP P0A0L5
B	103	TRP	THR	SEE REMARK 999	UNP P0A0L5
B	104	HIS	GLY	SEE REMARK 999	UNP P0A0L5
D	?	-	GLY	SEE REMARK 999	UNP P0A0L5
D	?	-	LYS	SEE REMARK 999	UNP P0A0L5
D	102	TRP	VAL	SEE REMARK 999	UNP P0A0L5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	103	TRP	THR	SEE REMARK 999	UNP P0A0L5
D	104	HIS	GLY	SEE REMARK 999	UNP P0A0L5
F	?	-	GLY	SEE REMARK 999	UNP P0A0L5
F	?	-	LYS	SEE REMARK 999	UNP P0A0L5
F	102	TRP	VAL	SEE REMARK 999	UNP P0A0L5
F	103	TRP	THR	SEE REMARK 999	UNP P0A0L5
F	104	HIS	GLY	SEE REMARK 999	UNP P0A0L5
H	?	-	GLY	SEE REMARK 999	UNP P0A0L5
H	?	-	LYS	SEE REMARK 999	UNP P0A0L5
H	102	TRP	VAL	SEE REMARK 999	UNP P0A0L5
H	103	TRP	THR	SEE REMARK 999	UNP P0A0L5
H	104	HIS	GLY	SEE REMARK 999	UNP P0A0L5

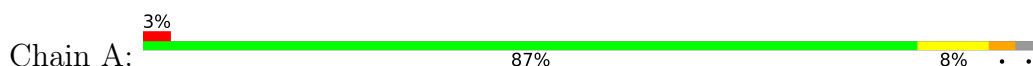
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	64	Total O 64 64	0	0
3	B	118	Total O 118 118	0	0
3	C	56	Total O 56 56	0	0
3	D	85	Total O 85 85	0	0
3	E	50	Total O 50 50	0	0
3	F	91	Total O 91 91	0	0
3	G	45	Total O 45 45	0	0
3	H	75	Total O 75 75	0	0

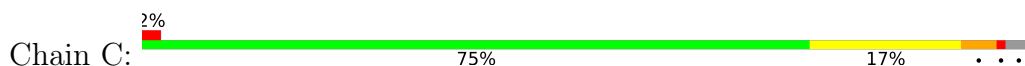
3 Residue-property plots [i](#)

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

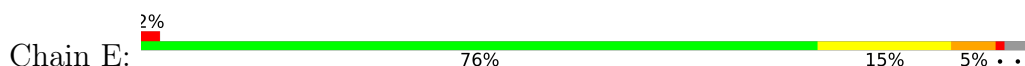
- Molecule 1: T-cell receptor beta chain V



- Molecule 1: T-cell receptor beta chain V



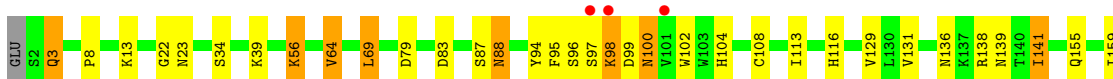
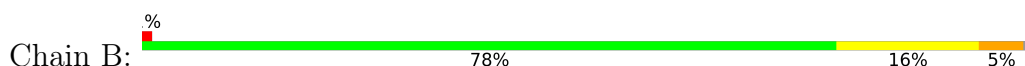
- Molecule 1: T-cell receptor beta chain V

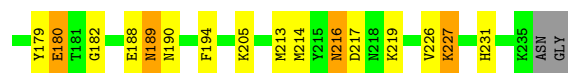


- Molecule 1: T-cell receptor beta chain V

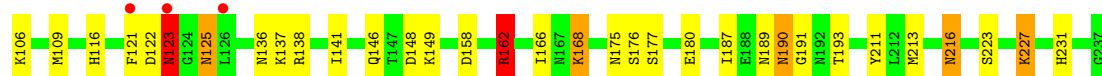
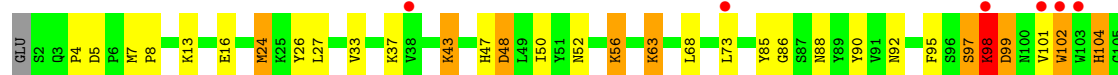
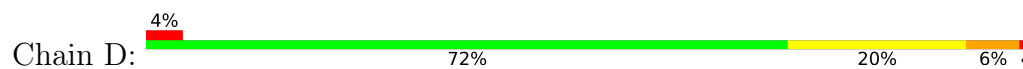


- Molecule 2: Enterotoxin type C-3

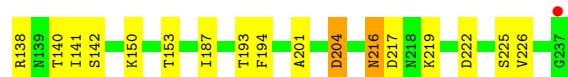
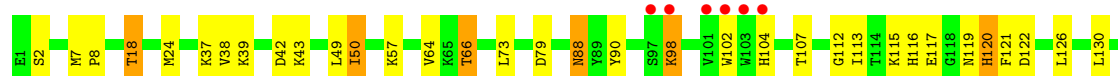
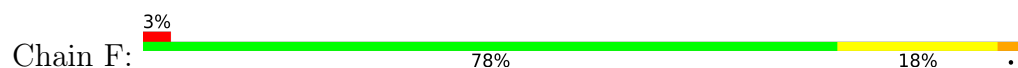




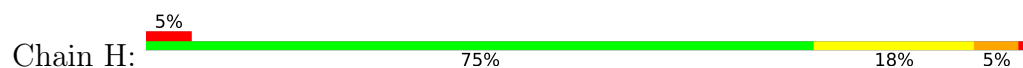
• Molecule 2: Enterotoxin type C-3



• Molecule 2: Enterotoxin type C-3



• Molecule 2: Enterotoxin type C-3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	63.20Å 70.19Å 98.40Å 74.79° 75.05° 88.54°	Depositor
Resolution (Å)	35.00 – 2.10 35.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	96.0 (35.00-2.10) 88.9 (35.00-2.10)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.95 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.185 , 0.243 0.195 , 0.197	Depositor DCC
R_{free} test set	4085 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.711	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11673	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 4.91% 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	1.67	2/850 (0.2%)	1.34	3/1153 (0.3%)
1	C	1.57	6/850 (0.7%)	1.40	7/1153 (0.6%)
1	E	1.58	7/850 (0.8%)	1.15	2/1153 (0.2%)
1	G	1.77	7/850 (0.8%)	1.23	2/1153 (0.2%)
2	B	1.36	8/1972 (0.4%)	1.16	3/2660 (0.1%)
2	D	1.24	2/1985 (0.1%)	1.14	9/2676 (0.3%)
2	F	1.30	6/1994 (0.3%)	1.15	4/2688 (0.1%)
2	H	1.25	4/1994 (0.2%)	1.16	8/2688 (0.3%)
All	All	1.40	42/11345 (0.4%)	1.19	38/15324 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
1	G	0	1
2	D	0	1
2	F	0	1
2	H	0	1
All	All	0	7

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	63	GLY	C-N	22.45	1.61	1.33
1	G	63	GLY	C-N	20.89	1.62	1.33
1	G	101	TYR	C-N	19.46	1.60	1.33
1	C	63	GLY	C-N	17.84	1.60	1.33
1	C	101	TYR	C-N	15.22	1.55	1.33
1	E	63	GLY	C-N	14.22	1.55	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	TYR	C-N	12.46	1.50	1.33
1	E	101	TYR	C-N	12.12	1.50	1.33
1	E	67	ALA	CA-CB	8.28	1.68	1.53
1	E	52	VAL	CA-CB	7.34	1.63	1.54
1	G	78	ILE	CA-CB	7.22	1.63	1.54
1	E	81	SER	CA-C	-6.73	1.47	1.53
2	B	131	VAL	CA-CB	6.26	1.62	1.54
2	H	163	ASN	C-O	6.17	1.31	1.24
1	G	69	ARG	CA-C	6.07	1.59	1.52
1	E	55	THR	CA-CB	6.02	1.64	1.53
2	F	24	MET	CA-C	5.97	1.60	1.52
1	G	60	ILE	CA-C	5.93	1.59	1.52
2	B	87	SER	CA-C	5.92	1.60	1.52
1	G	43	LEU	CA-C	-5.89	1.45	1.52
2	H	64	VAL	CA-CB	5.74	1.61	1.54
1	E	19	VAL	CA-C	5.67	1.59	1.52
2	B	56	LYS	C-O	5.65	1.29	1.23
2	H	230	VAL	CA-CB	5.60	1.60	1.54
2	B	22	GLY	N-CA	5.57	1.53	1.45
2	F	66	THR	CA-C	-5.53	1.45	1.52
2	B	226	VAL	CA-CB	5.53	1.60	1.54
2	D	26	TYR	CA-CB	5.44	1.61	1.53
2	H	172	TYR	CA-C	-5.43	1.46	1.52
2	F	18	THR	CA-CB	5.32	1.61	1.53
1	C	52	VAL	CA-CB	5.29	1.59	1.54
2	B	64	VAL	CA-CB	5.23	1.61	1.54
2	D	211	TYR	C-O	5.22	1.30	1.24
1	C	78	ILE	CA-CB	5.22	1.61	1.54
2	F	50	ILE	CA-CB	5.18	1.60	1.54
2	B	179	TYR	C-O	5.16	1.29	1.23
1	G	93	ALA	CA-CB	5.09	1.63	1.54
2	B	129	VAL	CA-CB	5.08	1.61	1.54
1	C	19	VAL	CA-CB	5.04	1.61	1.54
1	C	115	SER	CA-C	-5.04	1.46	1.52
2	F	226	VAL	N-CA	5.03	1.52	1.46
2	F	226	VAL	CA-CB	5.02	1.59	1.54

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	GLY	O-C-N	-18.02	102.95	122.41
1	C	63	GLY	CA-C-N	-10.85	105.69	122.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	63	GLY	C-N-CA	-10.85	105.69	122.62
1	C	101	TYR	O-C-N	-10.73	106.66	122.96
2	H	104	HIS	N-CA-C	7.90	124.06	108.18
1	E	63	GLY	O-C-N	-7.81	112.54	122.70
1	C	63	GLY	O-C-N	7.20	131.57	122.43
2	B	99	ASP	N-CA-C	-7.07	101.84	113.50
1	C	101	TYR	CA-C-N	6.88	133.84	122.07
1	C	101	TYR	C-N-CA	6.88	133.84	122.07
2	H	147	THR	CB-CA-C	-6.75	95.96	109.79
1	G	63	GLY	O-C-N	-6.61	114.73	122.60
2	D	99	ASP	N-CA-C	-6.45	105.38	113.18
2	H	124	GLY	N-CA-C	-6.35	107.13	114.69
1	A	27	ASN	N-CA-C	6.31	120.83	113.20
1	G	37	GLN	N-CA-C	6.29	118.69	108.63
2	D	162	ARG	NE-CZ-NH1	6.19	127.69	121.50
2	D	223	SER	N-CA-C	6.04	117.53	111.07
1	A	101	TYR	O-C-N	-5.89	115.36	123.01
2	F	120	HIS	N-CA-C	5.81	119.02	110.59
2	F	201	ALA	CA-C-N	5.74	126.06	119.92
2	F	201	ALA	C-N-CA	5.74	126.06	119.92
2	D	104	HIS	N-CA-C	5.73	118.81	109.24
2	B	180	GLU	N-CA-C	-5.65	106.05	113.12
2	D	48	ASP	N-CA-C	5.60	118.20	109.52
1	E	52	VAL	N-CA-CB	5.59	117.42	110.05
2	H	98	LYS	N-CA-C	-5.50	99.08	110.80
2	F	98	LYS	N-CA-C	-5.44	106.41	113.16
2	H	16	GLU	N-CA-C	5.38	119.69	113.18
2	H	230	VAL	CB-CA-C	5.30	118.05	110.84
1	C	27	ASN	N-CA-C	5.25	119.68	113.16
2	H	225	SER	N-CA-C	5.25	119.81	113.41
2	H	100	ASN	N-CA-C	5.24	118.12	108.58
2	D	97	SER	N-CA-C	-5.19	106.08	112.72
2	D	123	ASN	N-CA-C	5.10	116.56	108.96
2	D	175	ASN	N-CA-CB	-5.07	102.61	110.07
2	D	166	ILE	N-CA-C	-5.06	105.61	110.72
2	B	97	SER	N-CA-C	-5.01	106.75	112.92

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	101	TYR	Mainchain

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Mol	Chain	Res	Type	Group
1	A	63	GLY	Mainchain
1	C	101	TYR	Mainchain
2	D	98	LYS	Peptide
2	F	121	PHE	Peptide
1	G	63	GLY	Mainchain
2	H	97	SER	Peptide

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	832	0	793	8	0
1	C	832	0	793	12	0
1	E	832	0	793	19	0
1	G	832	0	793	19	0
2	B	1926	0	1854	32	0
2	D	1939	0	1863	51	0
2	F	1948	0	1872	31	0
2	H	1948	0	1872	30	0
3	A	64	0	0	1	0
3	B	118	0	0	3	0
3	C	56	0	0	0	0
3	D	85	0	0	9	0
3	E	50	0	0	3	0
3	F	91	0	0	6	0
3	G	45	0	0	4	0
3	H	75	0	0	2	0
All	All	11673	0	10633	193	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 9.

All (193) 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:24:MET:HA	2:D:24:MET:HE3	1.39	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:158:ASP:OD1	2:D:162:ARG:HD3	1.62	0.98
2:F:120:HIS:O	2:F:150:LYS:HE3	1.72	0.88
1:E:80:VAL:HG12	3:E:131:HOH:O	1.74	0.87
1:A:55:THR:H	2:B:23:ASN:HD21	1.21	0.86
2:D:24:MET:HA	2:D:24:MET:CE	2.06	0.84
2:D:158:ASP:O	2:D:162:ARG:HG2	1.79	0.81
2:B:100:ASN:HB3	2:B:102:TRP:HD1	1.44	0.81
2:F:88:ASN:HD22	2:F:88:ASN:H	1.27	0.80
2:D:92:ASN:HB2	3:D:296:HOH:O	1.79	0.80
2:H:88:ASN:H	2:H:88:ASN:HD22	1.30	0.79
2:D:168:LYS:HE3	2:D:168:LYS:HA	1.63	0.79
2:D:24:MET:HE1	2:D:27:LEU:HD12	1.62	0.79
2:H:227:LYS:HA	2:H:227:LYS:HE2	1.66	0.78
1:E:44:ARG:HG3	1:E:44:ARG:HH21	1.48	0.78
2:D:168:LYS:HE3	2:D:168:LYS:CA	2.12	0.78
1:G:42:GLY:HA2	3:G:148:HOH:O	1.82	0.77
2:B:213:MET:HE2	3:B:279:HOH:O	1.84	0.77
1:A:9:ARG:HB3	1:A:9:ARG:NH1	1.99	0.76
1:A:9:ARG:HB3	1:A:9:ARG:HH11	1.52	0.75
2:B:189:ASN:HD22	2:B:190:ASN:N	1.83	0.75
2:B:214:MET:HE3	3:B:283:HOH:O	1.87	0.73
2:D:138:ARG:HD3	3:D:273:HOH:O	1.88	0.73
2:B:100:ASN:HB3	2:B:102:TRP:CD1	2.25	0.72
2:H:102:TRP:HB2	2:H:104:HIS:HD2	1.55	0.72
2:D:136:ASN:O	2:D:137:LYS:HB2	1.90	0.71
2:B:205:LYS:HD3	3:B:289:HOH:O	1.91	0.71
2:H:13:LYS:HB3	2:H:180:GLU:OE1	1.91	0.71
2:D:56:LYS:CD	2:D:56:LYS:H	2.04	0.70
3:F:321:HOH:O	1:G:113:ARG:HB3	1.90	0.70
2:D:168:LYS:HA	2:D:168:LYS:CE	2.21	0.70
2:H:128:ASN:HB3	2:H:144:GLU:HG2	1.73	0.70
1:E:80:VAL:HG11	1:G:83:THR:CG2	2.23	0.69
1:G:28:ASN:ND2	1:G:72:GLN:HG2	2.07	0.68
1:E:57:LYS:HD2	3:F:294:HOH:O	1.92	0.67
1:G:21:LEU:HD22	1:G:112:THR:HG21	1.76	0.67
2:D:13:LYS:HB2	2:D:16:GLU:HG3	1.76	0.66
2:D:24:MET:CE	2:D:27:LEU:HD12	2.26	0.65
2:D:97:SER:C	2:D:99:ASP:H	2.03	0.65
2:H:202:PRO:HG3	3:H:312:HOH:O	1.97	0.65
2:H:101:VAL:O	2:H:102:TRP:HB2	1.98	0.64
2:H:147:THR:HG21	2:H:152:VAL:CG2	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:ARG:HB3	1:C:9:ARG:NH1	2.12	0.63
1:C:77:LEU:C	1:C:78:ILE:HD13	2.23	0.63
2:H:189:ASN:HD22	2:H:190:ASN:N	1.96	0.63
2:H:189:ASN:HD22	2:H:190:ASN:H	1.46	0.62
2:D:13:LYS:HB3	2:D:180:GLU:OE1	2.00	0.62
2:F:88:ASN:H	2:F:88:ASN:ND2	1.92	0.62
2:D:189:ASN:C	2:D:191:GLY:H	2.08	0.62
2:H:115:LYS:HG3	3:H:281:HOH:O	1.98	0.62
2:H:123:ASN:HB3	2:H:125:ASN:H	1.65	0.61
2:H:147:THR:HG21	2:H:152:VAL:HG21	1.81	0.61
2:F:66:THR:HG21	2:F:113:ILE:HD11	1.82	0.61
2:H:236:ASN:N	2:H:236:ASN:OD1	2.34	0.60
2:B:83:ASP:OD1	2:B:116:HIS:HD2	1.84	0.60
1:E:80:VAL:CG1	1:G:83:THR:HG21	2.31	0.60
1:E:80:VAL:HG11	1:G:83:THR:HG21	1.83	0.59
2:F:39:LYS:HD2	2:F:79:ASP:O	2.02	0.59
2:H:227:LYS:HA	2:H:227:LYS:CE	2.29	0.59
2:B:88:ASN:HD22	2:B:88:ASN:H	1.51	0.59
2:D:176:SER:OG	2:D:177:SER:N	2.31	0.59
2:D:123:ASN:HA	3:D:275:HOH:O	2.01	0.58
2:H:55:ASP:OD1	2:H:57:LYS:HG2	2.02	0.58
2:H:68:LEU:HD21	2:H:113:ILE:HD12	1.85	0.58
1:E:52:VAL:HG22	2:F:90:TYR:CD1	2.39	0.57
2:F:112:GLY:HA2	2:F:153:THR:HG21	1.85	0.57
2:D:24:MET:CE	2:D:24:MET:CA	2.80	0.57
2:B:189:ASN:HD22	2:B:190:ASN:H	1.51	0.56
2:F:88:ASN:HD22	2:F:88:ASN:N	2.01	0.56
1:C:52:VAL:HG22	2:D:90:TYR:CD1	2.40	0.56
2:D:47:HIS:H	2:D:47:HIS:CD2	2.25	0.55
2:F:104:HIS:HB3	3:F:328:HOH:O	2.06	0.55
2:B:94:TYR:O	2:B:95:PHE:HB3	2.06	0.54
1:E:80:VAL:CG1	1:G:83:THR:CG2	2.86	0.54
1:E:9:ARG:HH22	1:E:110:ALA:HB3	1.73	0.54
1:A:62:ASP:HB2	3:A:124:HOH:O	2.08	0.53
2:D:43:LYS:HA	2:D:50:ILE:HG12	1.89	0.53
2:D:92:ASN:CB	3:D:296:HOH:O	2.45	0.53
2:F:39:LYS:CD	2:F:79:ASP:O	2.57	0.53
2:F:138:ARG:HD2	2:F:140:THR:HG22	1.91	0.53
2:F:222:ASP:OD2	2:F:225:SER:OG	2.17	0.53
2:H:214:MET:HE3	2:H:215:TYR:CE2	2.44	0.53
2:H:88:ASN:H	2:H:88:ASN:ND2	2.04	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:31:ASN:ND2	1:G:50:TYR:HD1	2.07	0.52
2:F:187:ILE:HG23	2:F:193:THR:HG22	1.90	0.52
2:F:115:LYS:HE3	2:F:117:GLU:N	2.24	0.52
2:D:97:SER:C	2:D:99:ASP:N	2.68	0.51
2:F:18:THR:OG1	2:F:204:ASP:OD2	2.22	0.51
2:F:119:ASN:O	2:F:150:LYS:HG3	2.11	0.51
2:F:138:ARG:HD3	3:F:327:HOH:O	2.09	0.51
1:A:55:THR:H	2:B:23:ASN:ND2	2.00	0.51
2:D:168:LYS:CA	2:D:168:LYS:CE	2.86	0.51
2:H:147:THR:HB	2:H:149:LYS:H	1.76	0.50
2:F:115:LYS:HE3	2:F:117:GLU:HB2	1.94	0.50
1:G:22:SER:HB3	3:G:162:HOH:O	2.10	0.50
2:D:231:HIS:ND1	3:D:286:HOH:O	2.35	0.50
2:H:187:ILE:HB	2:H:227:LYS:HB3	1.94	0.50
2:F:115:LYS:CE	2:F:117:GLU:HB2	2.41	0.49
2:B:182:GLY:HA2	2:B:231:HIS:O	2.13	0.49
1:E:44:ARG:HH21	1:E:44:ARG:CG	2.21	0.49
3:E:149:HOH:O	1:G:84:PRO:HG2	2.12	0.49
2:H:77:TYR:O	2:H:78:LYS:C	2.56	0.49
2:B:194:PHE:CE2	2:B:219:LYS:HE2	2.48	0.49
2:H:214:MET:HE3	2:H:215:TYR:CZ	2.47	0.49
2:B:136:ASN:O	2:B:138:ARG:NH1	2.47	0.48
2:D:213:MET:O	2:D:216:ASN:HB2	2.13	0.48
2:F:117:GLU:CG	3:F:305:HOH:O	2.60	0.48
2:F:130:LEU:HD11	2:F:142:SER:HB3	1.94	0.48
2:D:37:LYS:HG3	2:D:116:HIS:CD2	2.49	0.48
1:A:24:GLN:OE1	1:A:74:GLN:NE2	2.44	0.48
1:C:57:LYS:HB3	1:C:61:PRO:HG3	1.96	0.48
2:F:7:MET:O	2:F:8:PRO:C	2.56	0.48
2:D:98:LYS:NZ	3:D:283:HOH:O	2.47	0.48
2:F:194:PHE:CE2	2:F:219:LYS:HE3	2.49	0.47
1:C:31:ASN:HA	1:C:49:SER:O	2.13	0.47
2:B:227:LYS:HA	2:B:227:LYS:HD2	1.68	0.47
2:B:213:MET:O	2:B:216:ASN:HB2	2.14	0.47
2:F:115:LYS:HE3	2:F:117:GLU:H	1.80	0.47
2:B:3:GLN:HE21	2:B:194:PHE:HB2	1.80	0.47
2:B:188:GLU:OE1	2:B:219:LYS:NZ	2.44	0.47
2:D:138:ARG:CD	3:D:273:HOH:O	2.54	0.47
2:B:96:SER:HB3	2:B:98:LYS:HG2	1.96	0.47
2:H:37:LYS:HG3	2:H:116:HIS:CD2	2.50	0.47
2:H:222:ASP:OD2	2:H:225:SER:OG	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:ASN:H	2:B:88:ASN:ND2	2.12	0.46
2:F:64:VAL:HG22	2:F:107:THR:HG22	1.97	0.46
2:D:148:ASP:OD2	2:D:149:LYS:HG3	2.15	0.46
2:F:37:LYS:HG3	2:F:116:HIS:CD2	2.50	0.46
2:D:95:PHE:CZ	2:D:106:LYS:HB2	2.51	0.46
2:F:120:HIS:O	2:F:150:LYS:CE	2.55	0.46
2:F:187:ILE:HA	2:F:193:THR:HG22	1.97	0.46
1:A:6:GLN:HB2	1:A:9:ARG:HH21	1.81	0.46
1:C:88:SER:OG	1:C:89:VAL:N	2.49	0.46
1:C:9:ARG:HB3	1:C:9:ARG:HH11	1.78	0.45
2:D:24:MET:O	2:D:24:MET:HE2	2.17	0.45
2:H:57:LYS:N	2:H:57:LYS:HD3	2.31	0.45
2:F:117:GLU:HG2	3:F:305:HOH:O	2.17	0.45
2:B:56:LYS:HD3	2:B:56:LYS:HA	1.82	0.45
2:D:187:ILE:HG23	2:D:193:THR:HG22	1.98	0.45
2:D:86:GLY:HA3	2:D:109:MET:HE3	1.98	0.44
2:D:121:PHE:C	2:D:123:ASN:H	2.25	0.44
1:E:33:TYR:OH	3:E:128:HOH:O	2.21	0.44
1:G:66:GLU:HB2	1:G:78:ILE:HB	2.00	0.44
2:H:147:THR:CG2	2:H:152:VAL:HG21	2.48	0.44
1:C:8:PRO:HG2	1:C:11:LYS:HB2	1.99	0.44
2:F:42:ASP:HB3	2:F:50:ILE:HB	2.00	0.44
1:E:80:VAL:HG11	1:G:83:THR:HG22	1.99	0.44
1:G:42:GLY:CA	3:G:148:HOH:O	2.52	0.44
2:B:13:LYS:HB3	2:B:180:GLU:OE1	2.18	0.43
2:B:39:LYS:HD2	2:B:79:ASP:O	2.18	0.43
1:G:69:ARG:HD2	1:G:74:GLN:O	2.18	0.43
2:D:189:ASN:OD1	2:D:190:ASN:N	2.51	0.43
2:D:43:LYS:NZ	2:D:48:ASP:O	2.38	0.43
2:D:227:LYS:NZ	3:D:319:HOH:O	2.52	0.43
1:E:73:GLU:H	1:E:73:GLU:CD	2.27	0.43
2:D:52:ASN:OD1	2:D:63:LYS:CD	2.66	0.43
2:D:123:ASN:HB2	2:D:125:ASN:OD1	2.19	0.43
2:F:216:ASN:HD22	2:F:217:ASP:N	2.15	0.43
1:C:72:GLN:HE21	1:C:72:GLN:HB3	1.21	0.42
2:D:146:GLN:HE21	2:D:146:GLN:HB2	1.61	0.42
1:E:93:ALA:HA	1:E:101:TYR:O	2.19	0.42
2:D:7:MET:HG2	3:D:303:HOH:O	2.18	0.42
1:G:9:ARG:HG2	3:G:160:HOH:O	2.19	0.42
2:B:88:ASN:HA	2:B:108:CYS:O	2.20	0.42
1:C:31:ASN:OD1	1:C:31:ASN:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3:GLN:HE21	2:H:194:PHE:HA	1.85	0.42
2:D:101:VAL:C	2:D:102:TRP:O	2.62	0.42
2:D:227:LYS:HD2	2:D:227:LYS:HA	1.73	0.42
1:E:9:ARG:NH2	1:E:111:GLY:O	2.53	0.42
2:B:69:LEU:HG	2:B:217:ASP:HA	2.02	0.41
2:B:141:ILE:H	2:B:141:ILE:HD13	1.84	0.41
2:D:162:ARG:HG2	2:D:162:ARG:H	1.78	0.41
1:E:14:VAL:O	1:E:15:THR:C	2.61	0.41
2:H:6:PRO:HD3	2:H:195:TRP:CE2	2.54	0.41
2:B:113:ILE:HD13	2:B:113:ILE:HG21	1.78	0.41
2:B:189:ASN:HD22	2:B:189:ASN:C	2.23	0.41
1:C:78:ILE:HD13	1:C:78:ILE:N	2.33	0.41
2:D:158:ASP:CG	2:D:162:ARG:HH11	2.27	0.41
1:G:87:SER:O	1:G:88:SER:HB2	2.21	0.41
1:C:73:GLU:H	1:C:73:GLU:CD	2.29	0.41
1:E:24:GLN:HG2	1:E:74:GLN:NE2	2.36	0.41
1:G:11:LYS:HE3	1:G:19:VAL:HG13	2.02	0.41
1:G:2:ALA:O	1:G:3:ALA:HB3	2.21	0.41
2:D:4:PRO:O	2:D:5:ASP:C	2.63	0.41
1:E:24:GLN:HA	1:E:73:GLU:O	2.21	0.41
2:B:8:PRO:O	2:B:13:LYS:NZ	2.46	0.41
1:A:57:LYS:HB3	1:A:61:PRO:HG3	2.02	0.40
1:E:37:GLN:HB2	1:E:43:LEU:CD1	2.51	0.40
2:B:155:GLN:O	2:B:159:ILE:HG13	2.21	0.40
2:D:33:VAL:O	2:D:85:TYR:HA	2.21	0.40
2:B:216:ASN:HD22	2:B:216:ASN:HA	1.45	0.40
2:D:56:LYS:H	2:D:56:LYS:HD3	1.83	0.40
2:H:38:VAL:O	2:H:82:VAL:HG22	2.22	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	107/112 (96%)	106 (99%)	1 (1%)	0	100	100
1	C	107/112 (96%)	104 (97%)	2 (2%)	1 (1%)	14	10
1	E	107/112 (96%)	104 (97%)	3 (3%)	0	100	100
1	G	107/112 (96%)	102 (95%)	4 (4%)	1 (1%)	14	10
2	B	232/237 (98%)	217 (94%)	13 (6%)	2 (1%)	14	10
2	D	234/237 (99%)	208 (89%)	21 (9%)	5 (2%)	5	2
2	F	235/237 (99%)	215 (92%)	18 (8%)	2 (1%)	14	10
2	H	235/237 (99%)	209 (89%)	22 (9%)	4 (2%)	7	3
All	All	1364/1396 (98%)	1265 (93%)	84 (6%)	15 (1%)	11	8

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	98	LYS
2	D	102	TRP
2	D	122	ASP
2	D	190	ASN
2	D	98	LYS
1	G	3	ALA
2	H	102	TRP
2	B	100	ASN
2	F	57	LYS
2	F	102	TRP
2	H	98	LYS
2	D	8	PRO
2	H	236	ASN
1	C	88	SER
2	H	3	GLN

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	90/93 (97%)	88 (98%)	2 (2%)	45	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	90/93 (97%)	81 (90%)	9 (10%)	7	5
1	E	90/93 (97%)	82 (91%)	8 (9%)	9	6
1	G	90/93 (97%)	87 (97%)	3 (3%)	33	37
2	B	217/219 (99%)	206 (95%)	11 (5%)	21	21
2	D	218/219 (100%)	202 (93%)	16 (7%)	13	10
2	F	219/219 (100%)	207 (94%)	12 (6%)	19	18
2	H	219/219 (100%)	194 (89%)	25 (11%)	5	3
All	All	1233/1248 (99%)	1147 (93%)	86 (7%)	14	11

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	22	SER
2	B	3	GLN
2	B	34	SER
2	B	64	VAL
2	B	69	LEU
2	B	88	ASN
2	B	104	HIS
2	B	139	ASN
2	B	141	ILE
2	B	189	ASN
2	B	216	ASN
2	B	227	LYS
1	C	14	VAL
1	C	24	GLN
1	C	43	LEU
1	C	52	VAL
1	C	72	GLN
1	C	73	GLU
1	C	80	VAL
1	C	83	THR
1	C	94	SER
2	D	24	MET
2	D	43	LYS
2	D	56	LYS
2	D	63	LYS
2	D	68	LEU
2	D	73	LEU

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Mol	Chain	Res	Type
2	D	88	ASN
2	D	98	LYS
2	D	104	HIS
2	D	123	ASN
2	D	125	ASN
2	D	141	ILE
2	D	162	ARG
2	D	168	LYS
2	D	216	ASN
2	D	227	LYS
1	E	9	ARG
1	E	10	ASN
1	E	14	VAL
1	E	18	LYS
1	E	24	GLN
1	E	43	LEU
1	E	44	ARG
1	E	52	VAL
2	F	2	SER
2	F	38	VAL
2	F	43	LYS
2	F	49	LEU
2	F	73	LEU
2	F	88	ASN
2	F	98	LYS
2	F	122	ASP
2	F	126	LEU
2	F	141	ILE
2	F	204	ASP
2	F	216	ASN
1	G	14	VAL
1	G	43	LEU
1	G	44	ARG
2	H	1	GLU
2	H	2	SER
2	H	3	GLN
2	H	9	ASP
2	H	45	LEU
2	H	47	HIS
2	H	56	LYS
2	H	57	LYS
2	H	68	LEU

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Mol	Chain	Res	Type
2	H	71	GLU
2	H	73	LEU
2	H	75	LYS
2	H	88	ASN
2	H	97	SER
2	H	100	ASN
2	H	104	HIS
2	H	117	GLU
2	H	144	GLU
2	H	147	THR
2	H	189	ASN
2	H	216	ASN
2	H	227	LYS
2	H	229	GLU
2	H	230	VAL
2	H	236	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	28	ASN
1	A	31	ASN
1	A	74	GLN
2	B	3	GLN
2	B	23	ASN
2	B	88	ASN
2	B	116	HIS
2	B	123	ASN
2	B	139	ASN
2	B	189	ASN
2	B	192	ASN
2	B	216	ASN
1	C	24	GLN
1	C	28	ASN
1	C	30	ASN
1	C	37	GLN
1	C	72	GLN
1	C	74	GLN
2	D	47	HIS
2	D	88	ASN
2	D	92	ASN

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Mol	Chain	Res	Type
2	D	104	HIS
2	D	123	ASN
2	D	127	GLN
2	D	128	ASN
2	D	139	ASN
2	D	146	GLN
2	D	167	ASN
2	D	170	ASN
2	D	216	ASN
2	D	236	ASN
1	E	28	ASN
1	E	37	GLN
1	E	74	GLN
2	F	88	ASN
2	F	92	ASN
2	F	127	GLN
2	F	146	GLN
2	F	216	ASN
1	G	28	ASN
1	G	31	ASN
2	H	3	GLN
2	H	88	ASN
2	H	104	HIS
2	H	139	ASN
2	H	170	ASN
2	H	189	ASN
2	H	216	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 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	G	1
1	A	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	G	63:GLY	C	65:TYR	N	1.63
1	A	63:GLY	C	65:TYR	N	1.61
1	C	63:GLY	C	65:TYR	N	1.60

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	109/112 (97%)	-0.12	3 (2%) 55 57	24, 35, 46, 56	0
1	C	109/112 (97%)	0.01	2 (1%) 67 70	29, 38, 51, 59	0
1	E	109/112 (97%)	0.07	2 (1%) 67 70	29, 43, 61, 72	0
1	G	109/112 (97%)	0.02	2 (1%) 67 70	26, 37, 54, 66	0
2	B	234/237 (98%)	-0.02	3 (1%) 75 77	25, 39, 64, 87	0
2	D	236/237 (99%)	0.35	9 (3%) 44 46	26, 48, 79, 92	0
2	F	237/237 (100%)	0.16	7 (2%) 52 55	27, 43, 81, 104	0
2	H	237/237 (100%)	0.34	11 (4%) 37 39	29, 49, 83, 101	0
All	All	1380/1396 (98%)	0.14	39 (2%) 55 57	24, 42, 73, 104	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	103	TRP	5.0
2	F	102	TRP	4.6
2	H	101	VAL	4.4
1	E	3	ALA	4.3
2	D	102	TRP	4.3
1	G	3	ALA	4.2
2	H	103	TRP	4.0
2	F	101	VAL	4.0
2	F	237	GLY	3.6
2	H	102	TRP	3.5
2	D	101	VAL	3.4
1	G	2	ALA	3.0
2	H	122	ASP	2.8
2	F	104	HIS	2.8
1	A	39	THR	2.7
2	D	103	TRP	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	2	ALA	2.6
2	D	98	LYS	2.6
1	C	38	ASP	2.6
2	H	236	ASN	2.6
2	H	237	GLY	2.5
2	B	97	SER	2.4
2	H	98	LYS	2.4
2	D	123	ASN	2.4
1	A	2	ALA	2.3
1	A	9	ARG	2.3
2	H	104	HIS	2.3
2	H	105	GLY	2.3
2	D	121	PHE	2.2
2	D	73	LEU	2.1
2	H	100	ASN	2.1
2	H	118	GLY	2.1
2	B	98	LYS	2.1
2	F	97	SER	2.1
1	E	2	ALA	2.1
2	D	126	LEU	2.1
2	B	101	VAL	2.1
2	D	38	VAL	2.1
2	F	98	LYS	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.