Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:02 PM GMT

PDB ID	:	1IGC
Title	:	IGG1 FAB FRAGMENT (MOPC21) COMPLEX WITH DOMAIN III OF PROTEIN G FROM STREPTOCOCCUS
Authors	:	Derrick, J.P.; Wigley, D.B.
Deposited on	:	1994-08-05
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

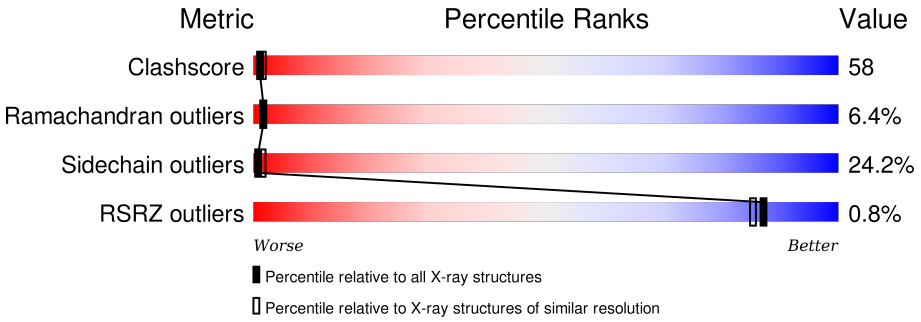
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 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	L	213	% 23% 41% 26% 9%
2	H	222	% 27% 44% 21% 8%
3	A	61	30% 48% 13% 5% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4117 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 IGG1-KAPPA MOPC21 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	0	0
			1651	1025	277	340	9			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	92	ASN	TYR	CONFLICT	UNP P01634
L	?	-	GLY	DELETION	UNP P01634

- Molecule 2 is a protein called IGG1-KAPPA MOPC21 FAB (HEAVY CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	222	Total	C	N	O	S	0	0	0
			1675	1057	281	327	10			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	5	VAL	LEU	CONFLICT	UNP P01783
H	13	GLN	LYS	CONFLICT	UNP P01783
H	18	ARG	LEU	CONFLICT	UNP P01783
H	31	SER	ASP	CONFLICT	UNP P01783
H	32	PHE	TYR	CONFLICT	UNP P01783
H	58	LEU	ILE	CONFLICT	UNP P01783
H	59	HIS	TYR	CONFLICT	UNP P01783
H	75	PRO	ALA	CONFLICT	UNP P01783
H	92	GLY	ALA	CONFLICT	UNP P01783
H	?	-	ASP	DELETION	UNP P01783
H	?	-	THR	DELETION	UNP P01783
H	?	-	THR	DELETION	UNP P01783
H	100	GLY	VAL	CONFLICT	UNP P01783
H	101	ASN	SER	CONFLICT	UNP P01783

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
H	102	TYR	GLY	CONFLICT	UNP P01783
H	103	PRO	HIS	CONFLICT	UNP P01783
H	106	ALA	VAL	CONFLICT	UNP P01783
H	194	PRO	THR	CONFLICT	UNP P01783
H	195	ARG	TRP	CONFLICT	UNP P01783
H	198	GLU	GLN	CONFLICT	UNP P01783

- Molecule 3 is a protein called STREPTOCOCCAL PROTEIN G (DOMAIN III).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	A	58	Total	C	N	O	0	0	0
			446	280	70	96			

- Molecule 4 is water.

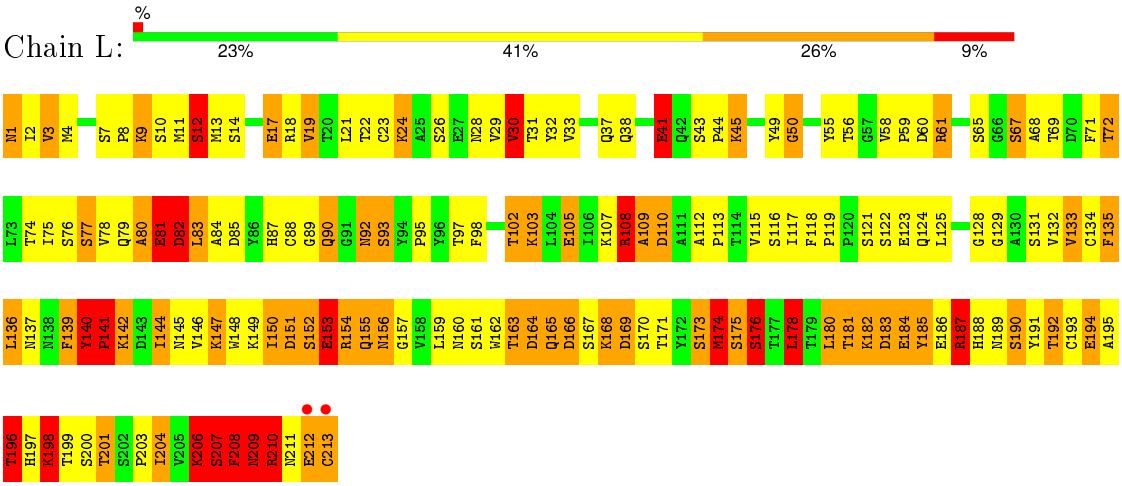
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	37	Total	O	0	0
			37	37		
4	H	145	Total	O	0	0
			145	145		
4	L	163	Total	O	0	0
			163	163		

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.

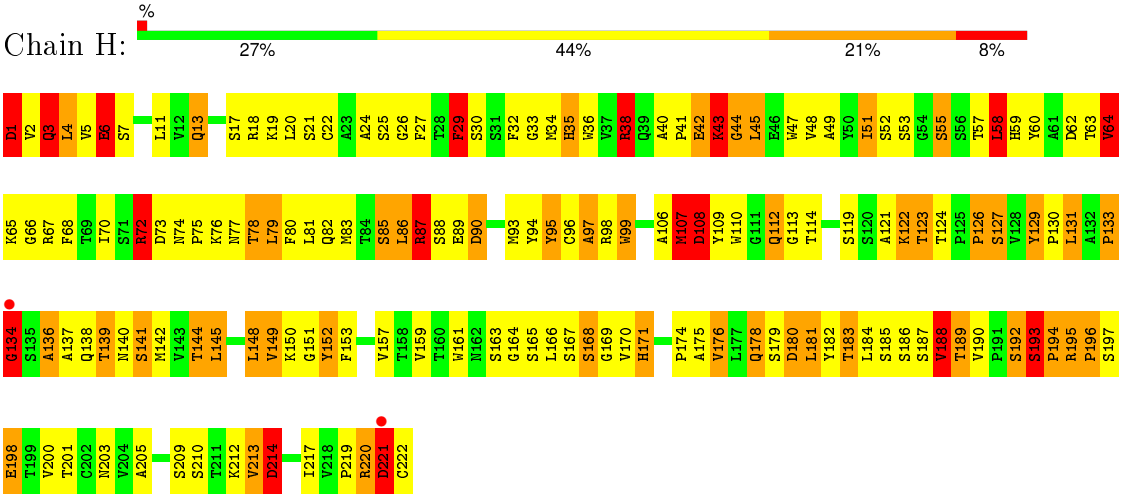
- Molecule 1: IGG1-KAPPA MOPC21 FAB (LIGHT CHAIN)

Chain L:



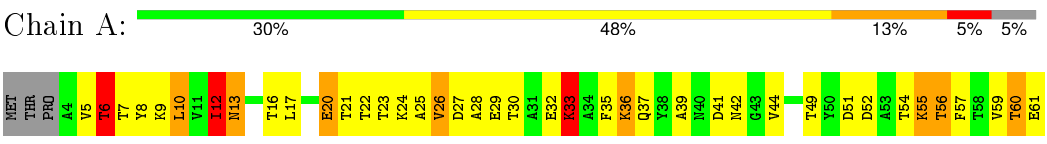
- Molecule 2: IGG1-KAPPA MOPC21 FAB (HEAVY CHAIN)

Chain H:



- Molecule 3: STREPTOCOCCAL PROTEIN G (DOMAIN III)

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.50Å 70.50Å 120.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 19.85 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.60) 98.7 (19.85-2.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.71 (at 2.59Å)	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.168 , (Not available) 0.167 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	35.8	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 188.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 17204 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4117	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	L	0.96	2/1687 (0.1%)	2.44	102/2291 (4.5%)
2	H	0.92	0/1722	2.55	92/2352 (3.9%)
3	A	0.87	0/452	2.13	15/613 (2.4%)
All	All	0.93	2/3861 (0.1%)	2.46	209/5256 (4.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	141	PRO	N-CD	6.99	1.57	1.47
1	L	30	VAL	N-CA	5.43	1.57	1.46

All (209) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	38	ARG	CD-NE-CZ	29.29	164.60	123.60
2	H	195	ARG	NE-CZ-NH1	27.18	133.89	120.30
2	H	67	ARG	CD-NE-CZ	24.61	158.05	123.60
1	L	141	PRO	N-CA-CB	19.39	126.57	103.30
2	H	195	ARG	CG-CD-NE	18.32	150.27	111.80
1	L	140	TYR	O-C-N	17.98	155.26	121.10
1	L	141	PRO	CA-N-CD	-16.95	87.77	111.50
2	H	67	ARG	NE-CZ-NH1	-15.32	112.64	120.30
1	L	140	TYR	C-N-CD	-14.27	89.21	120.60
1	L	210	ARG	NE-CZ-NH1	13.52	127.06	120.30
2	H	42	GLU	N-CA-CB	13.36	134.64	110.60
1	L	140	TYR	C-N-CA	13.06	176.86	122.00
1	L	210	ARG	CD-NE-CZ	12.47	141.06	123.60
2	H	195	ARG	NE-CZ-NH2	-12.42	114.09	120.30
1	L	210	ARG	NE-CZ-NH2	-11.98	114.31	120.30
1	L	141	PRO	N-CD-CG	11.89	121.03	103.20
1	L	133	VAL	CA-CB-CG1	11.00	127.40	110.90
1	L	207	SER	C-N-CA	10.37	147.62	121.70
2	H	72	ARG	NE-CZ-NH1	10.11	125.35	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	110	ASP	CB-CG-OD1	-10.03	109.27	118.30
2	H	98	ARG	NE-CZ-NH1	-10.02	115.29	120.30
2	H	89	GLU	OE1-CD-OE2	9.76	135.01	123.30
1	L	110	ASP	CB-CG-OD2	9.70	127.03	118.30
2	H	129	TYR	CB-CG-CD2	-9.58	115.25	121.00
1	L	153	GLU	C-N-CA	9.55	145.58	121.70
1	L	154	ARG	NE-CZ-NH2	-9.48	115.56	120.30
2	H	140	ASN	N-CA-CB	9.48	127.66	110.60
2	H	87	ARG	NE-CZ-NH1	9.23	124.91	120.30
2	H	95	TYR	CB-CG-CD2	9.11	126.47	121.00
2	H	18	ARG	NE-CZ-NH2	-8.98	115.81	120.30
2	H	42	GLU	CA-C-N	-8.94	97.53	117.20
2	H	98	ARG	CD-NE-CZ	-8.94	111.09	123.60
2	H	38	ARG	NE-CZ-NH2	8.90	124.75	120.30
2	H	195	ARG	CD-NE-CZ	8.70	135.77	123.60
2	H	43	LYS	CA-C-N	-8.59	99.01	116.20
1	L	206	LYS	C-N-CA	8.57	143.13	121.70
2	H	42	GLU	CA-C-O	8.53	138.00	120.10
1	L	152	SER	N-CA-CB	8.42	123.13	110.50
2	H	67	ARG	NE-CZ-NH2	8.41	124.51	120.30
2	H	133	PRO	C-N-CA	8.40	139.94	122.30
1	L	196	THR	N-CA-CB	8.31	126.09	110.30
2	H	194	PRO	CA-C-N	8.27	135.40	117.20
2	H	64	VAL	N-CA-CB	-8.24	93.36	111.50
2	H	129	TYR	CB-CG-CD1	8.08	125.85	121.00
2	H	43	LYS	C-N-CA	7.86	138.80	122.30
2	H	43	LYS	N-CA-CB	7.72	124.50	110.60
1	L	61	ARG	CD-NE-CZ	-7.68	112.85	123.60
2	H	171	HIS	N-CA-CB	7.67	124.40	110.60
1	L	154	ARG	N-CA-CB	-7.55	97.01	110.60
1	L	137	ASN	CA-CB-CG	7.43	129.75	113.40
3	A	20	GLU	CA-CB-CG	7.43	129.74	113.40
2	H	194	PRO	N-CA-C	7.27	131.00	112.10
3	A	6	THR	N-CA-CB	7.27	124.11	110.30
2	H	95	TYR	CB-CG-CD1	-7.26	116.64	121.00
1	L	154	ARG	N-CA-C	7.22	130.51	111.00
3	A	61	GLU	CG-CD-OE1	7.22	132.74	118.30
1	L	12	SER	N-CA-CB	7.21	121.32	110.50
1	L	1	ASN	CA-CB-CG	7.20	129.23	113.40
1	L	140	TYR	CA-C-O	-7.19	105.00	120.10
2	H	60	TYR	CB-CG-CD1	-7.19	116.69	121.00
1	L	169	ASP	CB-CG-OD2	7.16	124.74	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	190	SER	N-CA-CB	7.12	121.19	110.50
1	L	61	ARG	N-CA-CB	7.04	123.28	110.60
1	L	93	SER	N-CA-CB	-7.04	99.94	110.50
2	H	90	ASP	CB-CG-OD2	6.98	124.58	118.30
2	H	72	ARG	NE-CZ-NH2	-6.93	116.84	120.30
1	L	30	VAL	CB-CA-C	6.91	124.54	111.40
1	L	108	ARG	CG-CD-NE	-6.91	97.30	111.80
1	L	154	ARG	CD-NE-CZ	-6.89	113.96	123.60
3	A	56	THR	CA-CB-CG2	6.89	122.04	112.40
2	H	131	LEU	CB-CA-C	6.88	123.28	110.20
2	H	86	LEU	CB-CA-C	6.87	123.25	110.20
1	L	155	GLN	N-CA-C	6.85	129.51	111.00
2	H	127	SER	O-C-N	6.85	133.66	122.70
1	L	50	GLY	CA-C-N	6.84	132.26	117.20
2	H	89	GLU	CB-CA-C	-6.79	96.82	110.40
1	L	173	SER	N-CA-CB	6.78	120.67	110.50
2	H	29	PHE	CB-CG-CD1	6.74	125.52	120.80
2	H	195	ARG	NH1-CZ-NH2	-6.71	112.02	119.40
1	L	12	SER	CB-CA-C	-6.69	97.39	110.10
1	L	41	GLU	CA-C-O	6.67	134.10	120.10
2	H	220	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	L	166	ASP	CB-CG-OD1	6.63	124.27	118.30
1	L	187	ARG	NE-CZ-NH1	-6.56	117.02	120.30
1	L	41	GLU	C-N-CA	6.47	137.89	121.70
1	L	50	GLY	CA-C-O	-6.46	108.97	120.60
1	L	174	MET	CG-SD-CE	-6.43	89.92	100.20
2	H	212	LYS	N-CA-CB	6.42	122.17	110.60
1	L	176	SER	N-CA-CB	6.42	120.13	110.50
3	A	10	LEU	O-C-N	6.42	132.97	122.70
1	L	181	THR	N-CA-CB	6.41	122.49	110.30
2	H	44	GLY	CA-C-N	-6.35	103.22	117.20
3	A	12	ILE	O-C-N	6.34	132.85	122.70
1	L	41	GLU	CA-C-N	-6.34	103.26	117.20
2	H	89	GLU	CG-CD-OE2	-6.33	105.65	118.30
1	L	77	SER	O-C-N	6.31	132.80	122.70
2	H	3	GLN	N-CA-CB	6.31	121.95	110.60
2	H	174	PRO	N-CD-CG	-6.28	93.78	103.20
1	L	213	CYS	CA-CB-SG	6.27	125.28	114.00
1	L	140	TYR	CA-C-N	-6.25	99.61	117.10
1	L	37	GLN	CA-CB-CG	6.24	127.12	113.40
1	L	151	ASP	CB-CA-C	6.17	122.75	110.40
2	H	45	LEU	CB-CA-C	6.17	121.92	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	181	LEU	CB-CA-C	6.17	121.91	110.20
1	L	80	ALA	CB-CA-C	6.16	119.33	110.10
1	L	207	SER	N-CA-C	6.07	127.40	111.00
2	H	97	ALA	N-CA-CB	6.07	118.59	110.10
1	L	81	GLU	CB-CG-CD	6.06	130.56	114.20
1	L	81	GLU	CG-CD-OE1	6.06	130.41	118.30
2	H	59	HIS	N-CA-CB	6.01	121.42	110.60
2	H	6	GLU	CB-CG-CD	6.01	130.42	114.20
1	L	92	ASN	CB-CG-OD1	5.99	133.57	121.60
2	H	33	GLY	N-CA-C	-5.98	98.15	113.10
1	L	102	THR	N-CA-CB	5.98	121.66	110.30
1	L	163	THR	N-CA-CB	-5.96	98.97	110.30
2	H	108	ASP	CB-CG-OD1	5.95	123.65	118.30
1	L	1	ASN	N-CA-CB	5.93	121.28	110.60
2	H	220	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	L	140	TYR	CA-CB-CG	-5.92	102.15	113.40
2	H	149	VAL	O-C-N	5.91	132.16	122.70
3	A	56	THR	N-CA-CB	-5.90	99.10	110.30
2	H	221	ASP	C-N-CA	5.89	136.42	121.70
2	H	134	GLY	N-CA-C	5.86	127.74	113.10
1	L	164	ASP	CB-CA-C	5.85	122.10	110.40
2	H	221	ASP	CA-C-N	-5.79	104.46	117.20
1	L	140	TYR	N-CA-CB	5.78	121.00	110.60
1	L	135	PHE	CA-CB-CG	5.77	127.74	113.90
1	L	12	SER	O-C-N	5.76	131.92	122.70
2	H	188	VAL	CA-CB-CG2	5.74	119.51	110.90
1	L	50	GLY	N-CA-C	-5.74	98.75	113.10
2	H	59	HIS	O-C-N	5.74	131.88	122.70
2	H	35	HIS	CB-CA-C	-5.73	98.93	110.40
2	H	95	TYR	N-CA-CB	5.73	120.91	110.60
2	H	38	ARG	NH1-CZ-NH2	-5.71	113.11	119.40
1	L	164	ASP	CB-CG-OD1	5.70	123.43	118.30
2	H	60	TYR	CA-CB-CG	-5.70	102.58	113.40
1	L	151	ASP	CB-CG-OD2	5.68	123.42	118.30
1	L	38	GLN	CG-CD-OE1	5.68	132.97	121.60
1	L	109	ALA	CB-CA-C	5.68	118.62	110.10
1	L	201	THR	C-N-CA	5.68	135.91	121.70
1	L	83	LEU	CB-CA-C	5.66	120.96	110.20
1	L	209	ASN	CA-CB-CG	5.66	125.86	113.40
2	H	44	GLY	O-C-N	5.66	131.75	122.70
1	L	65	SER	N-CA-CB	5.63	118.95	110.50
2	H	171	HIS	O-C-N	5.63	131.71	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	194	GLU	CG-CD-OE1	-5.62	107.05	118.30
2	H	6	GLU	CG-CD-OE1	5.61	129.51	118.30
2	H	213	VAL	N-CA-CB	-5.57	99.25	111.50
3	A	33	LYS	N-CA-CB	5.56	120.60	110.60
2	H	221	ASP	CA-C-O	5.53	131.71	120.10
2	H	49	ALA	C-N-CA	5.52	135.51	121.70
2	H	45	LEU	N-CA-CB	-5.52	99.36	110.40
3	A	36	LYS	CA-CB-CG	5.52	125.54	113.40
1	L	204	ILE	N-CA-C	-5.51	96.13	111.00
1	L	3	VAL	C-N-CA	5.50	135.46	121.70
1	L	105	GLU	CA-CB-CG	5.50	125.49	113.40
3	A	13	ASN	N-CA-CB	5.49	120.48	110.60
3	A	22	THR	O-C-N	5.49	131.48	122.70
2	H	1	ASP	CB-CG-OD1	-5.47	113.38	118.30
2	H	152	TYR	CA-C-N	-5.47	105.17	117.20
2	H	198	GLU	CA-CB-CG	5.45	125.39	113.40
2	H	79	LEU	CB-CA-C	5.44	120.53	110.20
1	L	208	PHE	CA-CB-CG	5.43	126.94	113.90
1	L	174	MET	N-CA-CB	-5.38	100.91	110.60
1	L	23	CYS	CB-CA-C	5.37	121.15	110.40
2	H	214	ASP	N-CA-CB	5.37	120.26	110.60
2	H	32	PHE	O-C-N	5.35	132.30	123.20
1	L	110	ASP	N-CA-CB	5.33	120.19	110.60
1	L	153	GLU	O-C-N	-5.32	114.18	122.70
2	H	95	TYR	O-C-N	5.31	131.20	122.70
1	L	178	LEU	O-C-N	5.31	131.20	122.70
3	A	13	ASN	OD1-CG-ND2	5.30	134.08	121.90
1	L	164	ASP	N-CA-C	-5.29	96.72	111.00
2	H	152	TYR	CA-C-O	5.29	131.21	120.10
1	L	189	ASN	CA-CB-CG	5.28	125.01	113.40
1	L	49	TYR	CA-C-O	-5.24	109.11	120.10
3	A	41	ASP	CB-CG-OD2	5.22	123.00	118.30
3	A	41	ASP	CB-CG-OD1	-5.22	113.60	118.30
2	H	127	SER	N-CA-C	-5.22	96.91	111.00
1	L	154	ARG	NH1-CZ-NH2	5.21	125.13	119.40
2	H	3	GLN	O-C-N	5.20	131.03	122.70
1	L	137	ASN	CA-C-O	5.20	131.02	120.10
1	L	137	ASN	C-N-CA	5.19	134.68	121.70
1	L	49	TYR	CB-CA-C	5.18	120.77	110.40
2	H	198	GLU	CG-CD-OE2	-5.18	107.93	118.30
1	L	50	GLY	C-N-CA	-5.18	108.75	121.70
2	H	220	ARG	C-N-CA	5.16	134.61	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	16	THR	CA-CB-CG2	5.16	119.62	112.40
2	H	214	ASP	O-C-N	5.15	130.94	122.70
1	L	61	ARG	CB-CA-C	-5.15	100.11	110.40
1	L	166	ASP	N-CA-C	-5.15	97.11	111.00
1	L	108	ARG	NE-CZ-NH1	5.13	122.86	120.30
2	H	198	GLU	CB-CA-C	-5.12	100.16	110.40
1	L	129	GLY	O-C-N	5.11	130.88	122.70
1	L	165	GLN	O-C-N	5.11	130.88	122.70
2	H	32	PHE	CB-CA-C	-5.11	100.18	110.40
1	L	169	ASP	CB-CG-OD1	-5.09	113.71	118.30
2	H	43	LYS	CA-C-O	5.09	130.80	120.10
1	L	145	ASN	O-C-N	5.09	130.85	122.70
2	H	221	ASP	N-CA-C	5.09	124.75	111.00
2	H	66	GLY	C-N-CA	5.08	134.41	121.70
2	H	58	LEU	CA-CB-CG	5.07	126.95	115.30
2	H	42	GLU	CG-CD-OE1	5.05	128.41	118.30
1	L	107	LYS	N-CA-CB	5.01	119.63	110.60
1	L	81	GLU	OE1-CD-OE2	-5.01	117.28	123.30
1	L	74	THR	CA-C-O	-5.01	109.58	120.10
1	L	137	ASN	CA-C-N	-5.01	106.17	117.20
1	L	185	TYR	CA-C-N	-5.00	106.20	117.20
2	H	107	MET	C-N-CA	5.00	134.20	121.70

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	L	1651	0	1575	200	0
2	H	1675	0	1621	200	0
3	A	446	0	433	41	0
4	A	37	0	0	5	0
4	H	145	0	0	18	0
4	L	163	0	0	11	0
All	All	4117	0	3629	431	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 58.

All (431) 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:H:178:GLN:HE22	2:H:181:LEU:HB2	0.94	1.10
2:H:51:ILE:HD11	2:H:79:LEU:HD13	1.27	1.08
2:H:43:LYS:HG2	2:H:44:GLY:H	0.95	1.08
2:H:43:LYS:CG	2:H:44:GLY:H	1.55	1.08
2:H:193:SER:HB2	2:H:194:PRO:CD	1.83	1.07
2:H:193:SER:CB	2:H:194:PRO:HD3	1.85	1.07
2:H:196:PRO:HD2	2:H:197:SER:H	1.13	1.06
1:L:147:LYS:HG2	1:L:194:GLU:HB3	1.39	1.05
2:H:166:LEU:HB3	4:H:329:HOH:O	1.54	1.05
3:A:6:THR:HG22	3:A:25:ALA:O	1.56	1.05
1:L:8:PRO:O	1:L:9:LYS:HB2	1.57	1.02
2:H:43:LYS:HG2	2:H:44:GLY:N	1.74	1.02
1:L:163:THR:HG22	1:L:164:ASP:O	1.59	1.02
2:H:51:ILE:HD11	2:H:79:LEU:CD1	1.90	1.00
2:H:178:GLN:NE2	2:H:181:LEU:HB2	1.74	1.00
2:H:51:ILE:HG12	2:H:70:ILE:HG12	1.43	1.00
1:L:191:TYR:O	1:L:207:SER:O	1.80	0.99
1:L:18:ARG:HG3	1:L:76:SER:HA	1.41	0.98
2:H:193:SER:HB2	2:H:194:PRO:HD3	0.99	0.98
2:H:51:ILE:CD1	2:H:79:LEU:HD13	1.93	0.97
1:L:17:GLU:HB2	4:L:269:HOH:O	1.64	0.97
1:L:150:ILE:O	1:L:190:SER:O	1.84	0.95
1:L:17:GLU:HG3	1:L:18:ARG:N	1.77	0.95
2:H:87:ARG:HD2	2:H:88:SER:H	1.33	0.94
2:H:163:SER:H	2:H:203:ASN:ND2	1.65	0.94
1:L:13:MET:HG3	1:L:19:VAL:HG21	1.50	0.93
2:H:144:THR:HG21	4:H:275:HOH:O	1.67	0.93
1:L:150:ILE:CG2	1:L:151:ASP:H	1.83	0.91
2:H:163:SER:H	2:H:203:ASN:HD21	0.93	0.90
1:L:30:VAL:O	1:L:67:SER:O	1.89	0.90
1:L:69:THR:HG22	4:L:281:HOH:O	1.72	0.90
2:H:178:GLN:HE22	2:H:181:LEU:CB	1.83	0.90
3:A:27:ASP:HB2	3:A:30:THR:OG1	1.71	0.89
3:A:12:ILE:HD11	3:A:17:LEU:HD23	1.55	0.88
1:L:180:LEU:HD12	1:L:185:TYR:HB2	1.55	0.88
2:H:134:GLY:O	2:H:195:ARG:NH2	2.07	0.87
2:H:163:SER:N	2:H:203:ASN:HD21	1.73	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:62:ASP:HA	2:H:65:LYS:HE3	1.59	0.85
2:H:138:GLN:HG3	2:H:138:GLN:O	1.77	0.84
2:H:170:VAL:HG23	2:H:188:VAL:HG23	1.59	0.84
2:H:196:PRO:HD2	2:H:197:SER:N	1.93	0.84
2:H:196:PRO:CD	2:H:197:SER:H	1.89	0.83
1:L:30:VAL:CG2	1:L:31:THR:H	1.92	0.83
2:H:51:ILE:CG1	2:H:70:ILE:HG12	2.07	0.83
1:L:61:ARG:NH2	1:L:82:ASP:OD2	2.12	0.82
2:H:144:THR:HB	2:H:189:THR:HB	1.61	0.82
1:L:150:ILE:HG23	1:L:151:ASP:N	1.95	0.81
1:L:184:GLU:O	1:L:188:HIS:CD2	2.33	0.81
1:L:136:LEU:N	1:L:136:LEU:HD12	1.95	0.80
1:L:147:LYS:HD3	1:L:194:GLU:HG2	1.62	0.80
2:H:193:SER:CB	2:H:194:PRO:CD	2.51	0.80
3:A:6:THR:CG2	3:A:25:ALA:O	2.31	0.79
3:A:12:ILE:HB	3:A:59:VAL:HG12	1.64	0.78
1:L:83:LEU:HD21	1:L:165:GLN:HB2	1.65	0.78
2:H:170:VAL:CG2	2:H:188:VAL:HG23	2.14	0.78
1:L:110:ASP:OD2	1:L:198:LYS:HE3	1.85	0.77
2:H:34:MET:HB3	2:H:79:LEU:HD22	1.66	0.76
1:L:150:ILE:CG2	1:L:151:ASP:N	2.43	0.75
1:L:160:ASN:HD22	1:L:174:MET:HE3	1.51	0.75
1:L:147:LYS:CG	1:L:194:GLU:HB3	2.15	0.75
1:L:115:VAL:CG1	1:L:134:CYS:SG	2.75	0.75
1:L:160:ASN:ND2	1:L:174:MET:CE	2.49	0.75
1:L:41:GLU:OE1	1:L:41:GLU:HA	1.85	0.75
1:L:163:THR:CG2	1:L:164:ASP:O	2.35	0.75
1:L:160:ASN:ND2	1:L:174:MET:HE1	2.02	0.75
2:H:38:ARG:HG3	2:H:48:VAL:HG21	1.69	0.74
2:H:121:ALA:HB2	4:H:362:HOH:O	1.86	0.74
2:H:38:ARG:HG3	2:H:48:VAL:CG2	2.19	0.73
2:H:76:LYS:O	2:H:78:THR:HG23	1.87	0.73
1:L:166:ASP:N	1:L:171:THR:O	2.19	0.73
1:L:186:GLU:O	1:L:210:ARG:NH2	2.22	0.73
1:L:13:MET:HG3	1:L:19:VAL:CG2	2.18	0.73
2:H:145:LEU:HD12	2:H:188:VAL:HG12	1.71	0.73
2:H:180:ASP:O	2:H:181:LEU:HG	1.88	0.72
2:H:87:ARG:HD2	2:H:88:SER:N	2.05	0.72
1:L:142:LYS:O	1:L:162:TRP:CZ3	2.43	0.72
2:H:142:MET:HB3	4:H:282:HOH:O	1.90	0.71
1:L:212:GLU:HG2	4:L:305:HOH:O	1.90	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:87:HIS:ND1	4:L:216:HOH:O	2.23	0.71
2:H:79:LEU:HD12	2:H:80:PHE:H	1.55	0.71
1:L:61:ARG:HH22	1:L:82:ASP:CG	1.94	0.71
1:L:13:MET:HE2	1:L:19:VAL:HG23	1.73	0.70
2:H:99:TRP:O	2:H:108:ASP:HB2	1.91	0.70
1:L:30:VAL:HG22	1:L:31:THR:H	1.55	0.70
1:L:21:LEU:O	1:L:72:THR:HA	1.92	0.70
1:L:193:CYS:HB3	1:L:206:LYS:HB2	1.74	0.70
2:H:97:ALA:HB3	2:H:107:MET:HG2	1.73	0.70
2:H:166:LEU:C	4:H:329:HOH:O	2.28	0.70
1:L:83:LEU:HD23	1:L:167:SER:HA	1.74	0.69
3:A:52:ASP:O	3:A:55:LYS:HE2	1.92	0.69
2:H:175:ALA:HB1	2:H:182:TYR:HB3	1.74	0.69
1:L:95:PRO:HG3	4:H:268:HOH:O	1.92	0.69
1:L:21:LEU:HD22	1:L:102:THR:HG21	1.75	0.69
1:L:139:PHE:HZ	1:L:174:MET:HB2	1.58	0.69
1:L:33:VAL:O	1:L:50:GLY:O	2.10	0.69
1:L:185:TYR:CZ	1:L:210:ARG:HD3	2.27	0.69
1:L:108:ARG:NH1	1:L:109:ALA:O	2.25	0.69
1:L:185:TYR:CE2	1:L:210:ARG:HD3	2.28	0.69
1:L:142:LYS:O	1:L:162:TRP:CH2	2.45	0.69
1:L:8:PRO:O	1:L:9:LYS:CB	2.38	0.69
3:A:60:THR:CG2	4:A:98:HOH:O	2.38	0.68
2:H:157:VAL:CG2	2:H:184:LEU:HD21	2.23	0.68
2:H:94:TYR:O	2:H:113:GLY:HA2	1.94	0.68
1:L:79:GLN:HG2	1:L:80:ALA:N	2.09	0.68
2:H:51:ILE:HG12	2:H:70:ILE:CG1	2.22	0.68
1:L:150:ILE:HG22	1:L:151:ASP:H	1.58	0.67
1:L:8:PRO:HG3	1:L:11:MET:CE	2.25	0.67
1:L:133:VAL:HG11	2:H:131:LEU:HD13	1.77	0.67
1:L:43:SER:HB3	2:H:95:TYR:CE2	2.29	0.67
2:H:13:GLN:HB2	4:H:343:HOH:O	1.95	0.67
2:H:3:GLN:HG3	2:H:25:SER:OG	1.95	0.66
2:H:196:PRO:HB3	2:H:219:PRO:HG3	1.77	0.66
1:L:156:ASN:HD22	1:L:157:GLY:N	1.94	0.66
2:H:152:TYR:OH	2:H:184:LEU:HD23	1.95	0.66
1:L:139:PHE:O	1:L:140:TYR:CB	2.42	0.66
2:H:93:MET:HE2	2:H:113:GLY:HA3	1.77	0.66
2:H:145:LEU:HD13	2:H:200:VAL:HG11	1.78	0.66
1:L:160:ASN:HD22	1:L:174:MET:CE	2.09	0.66
1:L:182:LYS:HB3	1:L:182:LYS:NZ	2.11	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:161:TRP:HZ3	2:H:217:ILE:HD12	1.60	0.66
1:L:156:ASN:C	1:L:156:ASN:HD22	2.00	0.65
2:H:153:PHE:C	2:H:153:PHE:CD1	2.69	0.65
2:H:145:LEU:CD1	2:H:200:VAL:HG11	2.27	0.65
2:H:119:SER:O	4:H:237:HOH:O	2.14	0.65
1:L:30:VAL:CG2	1:L:31:THR:N	2.60	0.65
2:H:2:VAL:HG22	2:H:27:PHE:HB3	1.79	0.65
2:H:150:LYS:HA	2:H:183:THR:HB	1.79	0.65
2:H:99:TRP:O	2:H:106:ALA:O	2.15	0.65
1:L:8:PRO:HG3	1:L:11:MET:HE2	1.79	0.64
2:H:34:MET:CB	2:H:79:LEU:HD22	2.27	0.64
1:L:90:GLN:HE22	1:L:92:ASN:H	1.43	0.64
1:L:139:PHE:O	1:L:140:TYR:HB2	1.98	0.64
2:H:178:GLN:HE21	2:H:179:SER:H	1.45	0.64
2:H:74:ASN:N	2:H:75:PRO:HD2	2.13	0.64
3:A:6:THR:HG23	3:A:8:TYR:CE2	2.33	0.63
2:H:209:SER:O	2:H:210:SER:OG	2.17	0.63
2:H:38:ARG:HG2	2:H:94:TYR:CE2	2.34	0.63
4:L:233:HOH:O	2:H:110:TRP:HD1	1.79	0.63
3:A:13:ASN:HB3	4:A:64:HOH:O	1.98	0.63
2:H:157:VAL:HG22	2:H:184:LEU:HD21	1.79	0.63
1:L:178:LEU:HD11	1:L:180:LEU:HD23	1.80	0.63
2:H:152:TYR:CE2	2:H:157:VAL:HG13	2.34	0.63
1:L:115:VAL:HG12	1:L:206:LYS:HG2	1.81	0.63
1:L:169:ASP:O	1:L:171:THR:N	2.31	0.62
2:H:151:GLY:O	2:H:181:LEU:HD22	1.98	0.62
1:L:61:ARG:NH2	1:L:82:ASP:CG	2.53	0.62
2:H:35:HIS:CG	2:H:107:MET:HE2	2.35	0.61
1:L:128:GLY:HA2	1:L:182:LYS:HD3	1.83	0.61
2:H:13:GLN:HG3	4:H:345:HOH:O	2.00	0.61
1:L:2:ILE:HD13	1:L:29:VAL:HG12	1.83	0.61
3:A:27:ASP:CB	3:A:30:THR:OG1	2.46	0.61
1:L:144:ILE:HG22	1:L:162:TRP:CH2	2.36	0.61
1:L:110:ASP:OD2	1:L:141:PRO:HD3	2.01	0.61
2:H:43:LYS:CG	2:H:44:GLY:N	2.40	0.60
3:A:26:VAL:HG22	3:A:27:ASP:H	1.66	0.60
1:L:169:ASP:CG	1:L:169:ASP:O	2.39	0.60
1:L:121:SER:O	1:L:125:LEU:HG	2.02	0.59
1:L:132:VAL:N	1:L:178:LEU:O	2.34	0.59
2:H:20:LEU:HD13	2:H:114:THR:CG2	2.33	0.59
1:L:90:GLN:NE2	1:L:92:ASN:H	2.00	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:150:ILE:HG23	1:L:151:ASP:H	1.55	0.59
1:L:192:THR:HA	1:L:206:LYS:O	2.02	0.59
3:A:28:ALA:O	3:A:57:PHE:HZ	1.85	0.59
2:H:35:HIS:HD2	2:H:47:TRP:NE1	2.01	0.59
3:A:5:VAL:HG22	3:A:25:ALA:O	2.03	0.59
2:H:51:ILE:CG1	2:H:70:ILE:CG1	2.81	0.58
1:L:124:GLN:OE1	1:L:131:SER:HB2	2.02	0.58
2:H:112:GLN:HA	2:H:112:GLN:HE21	1.67	0.58
2:H:35:HIS:O	2:H:96:CYS:HA	2.03	0.58
2:H:163:SER:N	2:H:203:ASN:ND2	2.40	0.58
1:L:90:GLN:C	1:L:90:GLN:NE2	2.57	0.58
1:L:136:LEU:N	1:L:136:LEU:CD1	2.64	0.58
3:A:32:GLU:HA	3:A:35:PHE:HB2	1.84	0.58
2:H:35:HIS:HD2	2:H:47:TRP:HE1	1.49	0.58
2:H:195:ARG:N	2:H:196:PRO:HD3	2.18	0.58
2:H:196:PRO:CD	2:H:197:SER:N	2.56	0.57
2:H:38:ARG:NH1	2:H:90:ASP:HA	2.19	0.57
1:L:108:ARG:HG2	1:L:109:ALA:N	2.19	0.57
2:H:136:ALA:O	2:H:138:GLN:N	2.38	0.57
2:H:209:SER:C	2:H:210:SER:OG	2.44	0.57
1:L:159:LEU:HD22	2:H:176:VAL:HG21	1.87	0.56
2:H:40:ALA:HB1	2:H:41:PRO:CD	2.34	0.56
1:L:17:GLU:HG3	1:L:18:ARG:H	1.69	0.56
3:A:26:VAL:CG2	3:A:27:ASP:N	2.67	0.56
1:L:148:TRP:O	1:L:154:ARG:HA	2.06	0.56
1:L:178:LEU:CD1	1:L:180:LEU:HD23	2.36	0.56
3:A:26:VAL:CG2	3:A:27:ASP:H	2.19	0.56
2:H:127:SER:HA	3:A:42:ASN:HD21	1.71	0.56
2:H:74:ASN:N	2:H:75:PRO:CD	2.68	0.56
1:L:22:THR:HG22	1:L:24:LYS:HE2	1.86	0.56
2:H:51:ILE:CD1	2:H:70:ILE:HG12	2.36	0.56
2:H:131:LEU:HD21	2:H:148:LEU:HD12	1.88	0.56
2:H:36:TRP:HD1	2:H:70:ILE:HD12	1.69	0.56
1:L:147:LYS:HD3	1:L:194:GLU:CG	2.33	0.55
1:L:22:THR:CG2	1:L:24:LYS:HE2	2.36	0.55
2:H:134:GLY:C	2:H:195:ARG:NH2	2.59	0.55
1:L:33:VAL:HA	1:L:89:GLY:O	2.06	0.55
1:L:166:ASP:OD1	1:L:168:LYS:HG3	2.07	0.55
2:H:11:LEU:HD11	2:H:119:SER:HB3	1.88	0.55
3:A:32:GLU:O	3:A:36:LYS:HG2	2.06	0.55
2:H:6:GLU:HA	2:H:21:SER:O	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:74:ASN:HB2	2:H:75:PRO:HD3	1.89	0.55
3:A:8:TYR:CE2	3:A:25:ALA:HB3	2.42	0.55
1:L:108:ARG:NH1	1:L:108:ARG:HG2	2.21	0.55
2:H:51:ILE:HG13	2:H:70:ILE:CD1	2.37	0.55
2:H:122:LYS:HZ1	2:H:123:THR:HG23	1.72	0.55
1:L:108:ARG:HH11	1:L:108:ARG:HG2	1.73	0.54
2:H:11:LEU:HD23	2:H:123:THR:HG22	1.89	0.54
2:H:189:THR:HG22	4:H:276:HOH:O	2.07	0.54
2:H:51:ILE:CG1	2:H:70:ILE:CD1	2.86	0.54
1:L:115:VAL:HG12	1:L:134:CYS:SG	2.48	0.54
2:H:97:ALA:CB	2:H:107:MET:HG2	2.37	0.54
1:L:196:THR:HG23	1:L:203:PRO:HA	1.89	0.54
4:L:216:HOH:O	2:H:44:GLY:HA3	2.09	0.53
1:L:182:LYS:O	1:L:186:GLU:CG	2.56	0.53
2:H:139:THR:OG1	2:H:141:SER:N	2.40	0.53
3:A:37:GLN:HG3	3:A:37:GLN:O	2.09	0.53
2:H:141:SER:O	2:H:192:SER:OG	2.20	0.53
2:H:168:SER:OG	2:H:169:GLY:N	2.38	0.53
2:H:38:ARG:HB3	2:H:94:TYR:CD2	2.44	0.53
1:L:183:ASP:HA	1:L:186:GLU:HB2	1.90	0.53
2:H:35:HIS:CG	2:H:107:MET:CE	2.92	0.53
1:L:115:VAL:CG1	1:L:206:LYS:HG2	2.39	0.52
1:L:79:GLN:CG	1:L:80:ALA:N	2.72	0.52
1:L:133:VAL:HG11	2:H:131:LEU:CD1	2.39	0.52
2:H:43:LYS:HG2	2:H:44:GLY:CA	2.37	0.52
2:H:97:ALA:HA	2:H:109:TYR:O	2.10	0.52
2:H:42:GLU:HG3	2:H:43:LYS:N	2.24	0.52
1:L:180:LEU:HD13	1:L:185:TYR:HA	1.91	0.52
1:L:30:VAL:HG23	1:L:31:THR:H	1.70	0.52
1:L:32:TYR:O	1:L:90:GLN:HA	2.10	0.52
3:A:49:THR:HG23	4:A:98:HOH:O	2.10	0.52
1:L:147:LYS:CD	1:L:194:GLU:HB3	2.39	0.52
3:A:9:LYS:O	3:A:56:THR:HA	2.09	0.52
2:H:161:TRP:CZ3	2:H:217:ILE:HD12	2.45	0.51
2:H:219:PRO:C	2:H:221:ASP:H	2.13	0.51
2:H:1:ASP:O	2:H:26:GLY:HA3	2.09	0.51
2:H:180:ASP:C	2:H:181:LEU:HG	2.30	0.51
2:H:195:ARG:N	2:H:196:PRO:CD	2.73	0.51
1:L:45:LYS:HD3	4:L:231:HOH:O	2.11	0.51
1:L:136:LEU:HD23	1:L:144:ILE:CD1	2.40	0.51
1:L:115:VAL:HG13	1:L:134:CYS:SG	2.50	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:68:PHE:HB3	2:H:81:LEU:HD11	1.92	0.51
1:L:79:GLN:HG2	1:L:81:GLU:H	1.76	0.51
1:L:116:SER:O	1:L:134:CYS:HA	2.10	0.51
2:H:2:VAL:HG13	2:H:27:PHE:CD1	2.46	0.51
2:H:5:VAL:O	2:H:5:VAL:HG23	2.10	0.51
2:H:93:MET:HE3	2:H:113:GLY:C	2.30	0.51
3:A:60:THR:HG22	4:A:98:HOH:O	2.07	0.51
2:H:79:LEU:HD12	2:H:80:PHE:N	2.24	0.50
2:H:201:THR:CG2	2:H:214:ASP:HB3	2.41	0.50
2:H:6:GLU:N	2:H:6:GLU:OE1	2.42	0.50
2:H:35:HIS:HD2	2:H:47:TRP:CD1	2.30	0.50
2:H:35:HIS:CD2	2:H:47:TRP:HE1	2.28	0.50
1:L:115:VAL:O	1:L:206:LYS:HE2	2.11	0.50
1:L:149:LYS:HB3	1:L:154:ARG:HG2	1.92	0.49
1:L:196:THR:HG23	1:L:203:PRO:CA	2.42	0.49
2:H:178:GLN:NE2	2:H:179:SER:H	2.09	0.49
1:L:135:PHE:CE2	2:H:187:SER:HB3	2.47	0.49
1:L:150:ILE:HD13	1:L:155:GLN:NE2	2.27	0.49
2:H:68:PHE:CE1	2:H:83:MET:HB3	2.48	0.49
2:H:73:ASP:OD2	2:H:76:LYS:HD3	2.12	0.49
2:H:24:ALA:HB1	2:H:27:PHE:CE1	2.47	0.49
1:L:8:PRO:HG3	1:L:11:MET:HE3	1.93	0.49
2:H:43:LYS:HD3	2:H:44:GLY:O	2.13	0.49
1:L:147:LYS:HG2	1:L:194:GLU:CB	2.26	0.49
2:H:72:ARG:CD	2:H:74:ASN:OD1	2.61	0.49
1:L:150:ILE:N	1:L:153:GLU:O	2.43	0.49
1:L:139:PHE:O	1:L:171:THR:HG22	2.13	0.49
1:L:175:SER:O	1:L:175:SER:OG	2.29	0.49
1:L:159:LEU:HD13	2:H:176:VAL:HG22	1.94	0.49
1:L:160:ASN:OD1	1:L:176:SER:HB3	2.12	0.48
2:H:83:MET:HE1	2:H:94:TYR:CZ	2.48	0.48
1:L:195:ALA:O	1:L:204:ILE:HD12	2.12	0.48
3:A:27:ASP:HB2	3:A:30:THR:HG1	1.77	0.48
2:H:51:ILE:HG22	2:H:55:SER:HA	1.95	0.48
1:L:163:THR:HG23	4:L:288:HOH:O	2.12	0.48
1:L:108:ARG:HD3	1:L:109:ALA:O	2.14	0.48
2:H:34:MET:HB3	2:H:79:LEU:CD2	2.39	0.48
2:H:76:LYS:O	2:H:78:THR:CG2	2.57	0.48
1:L:2:ILE:O	1:L:97:THR:HG21	2.13	0.48
2:H:214:ASP:O	3:A:17:LEU:HA	2.14	0.48
2:H:19:LYS:HE3	2:H:80:PHE:CD2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:138:GLN:CG	2:H:138:GLN:O	2.54	0.47
1:L:81:GLU:O	1:L:83:LEU:N	2.46	0.47
1:L:206:LYS:HA	1:L:206:LYS:HD2	1.41	0.47
2:H:38:ARG:HH12	2:H:90:ASP:HA	1.79	0.47
1:L:43:SER:HB2	1:L:44:PRO:CD	2.43	0.47
1:L:163:THR:HB	1:L:173:SER:H	1.78	0.47
2:H:141:SER:O	2:H:192:SER:N	2.47	0.47
3:A:6:THR:O	3:A:25:ALA:N	2.36	0.47
3:A:59:VAL:HG13	3:A:59:VAL:O	2.13	0.47
3:A:29:GLU:O	3:A:33:LYS:HD3	2.14	0.47
1:L:103:LYS:HG3	4:L:329:HOH:O	2.14	0.47
2:H:161:TRP:HZ3	2:H:217:ILE:CD1	2.27	0.47
2:H:63:THR:HG23	2:H:64:VAL:HG23	1.96	0.47
3:A:51:ASP:OD1	3:A:54:THR:HG23	2.15	0.47
1:L:185:TYR:HA	1:L:191:TYR:OH	2.14	0.47
1:L:133:VAL:HG21	2:H:148:LEU:HD12	1.96	0.47
2:H:3:GLN:CG	2:H:25:SER:OG	2.61	0.47
2:H:129:TYR:HB2	2:H:148:LEU:HB3	1.97	0.47
2:H:122:LYS:HZ3	2:H:123:THR:H	1.63	0.47
1:L:2:ILE:HD13	1:L:29:VAL:CG1	2.45	0.47
1:L:197:HIS:C	1:L:199:THR:H	2.18	0.47
1:L:3:VAL:H	1:L:26:SER:HB3	1.79	0.47
2:H:178:GLN:HE21	2:H:179:SER:N	2.12	0.47
2:H:55:SER:HB3	4:H:253:HOH:O	2.15	0.47
3:A:12:ILE:CD1	3:A:44:VAL:HG21	2.44	0.47
1:L:83:LEU:CD2	1:L:165:GLN:HB2	2.42	0.47
2:H:25:SER:HB3	4:H:286:HOH:O	2.15	0.47
2:H:93:MET:HE2	2:H:113:GLY:CA	2.45	0.46
2:H:35:HIS:CD2	2:H:47:TRP:CD1	3.03	0.46
1:L:160:ASN:HB3	1:L:174:MET:CE	2.46	0.46
2:H:40:ALA:HB1	2:H:41:PRO:HD2	1.97	0.46
2:H:52:SER:N	2:H:57:THR:O	2.45	0.46
2:H:170:VAL:HG22	2:H:188:VAL:HG23	1.94	0.46
1:L:117:ILE:HD12	1:L:148:TRP:CZ3	2.50	0.46
1:L:182:LYS:HB3	1:L:182:LYS:HZ3	1.80	0.46
1:L:79:GLN:HG2	1:L:80:ALA:H	1.79	0.46
2:H:36:TRP:HD1	2:H:70:ILE:CD1	2.29	0.46
1:L:30:VAL:C	1:L:67:SER:O	2.51	0.46
2:H:138:GLN:HA	4:H:274:HOH:O	2.15	0.46
1:L:58:VAL:HA	1:L:59:PRO:HD3	1.80	0.46
2:H:52:SER:OG	2:H:57:THR:N	2.42	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:58:LEU:HD23	4:H:351:HOH:O	2.16	0.46
3:A:10:LEU:HG	3:A:12:ILE:HG22	1.98	0.46
2:H:72:ARG:HD2	2:H:74:ASN:OD1	2.16	0.46
3:A:5:VAL:HG13	3:A:24:LYS:HB3	1.98	0.46
1:L:28:ASN:ND2	1:L:68:ALA:HB1	2.30	0.46
1:L:55:TYR:CG	1:L:56:THR:N	2.84	0.45
2:H:176:VAL:HG13	4:H:279:HOH:O	2.16	0.45
2:H:124:THR:CG2	2:H:151:GLY:O	2.64	0.45
1:L:59:PRO:C	1:L:61:ARG:H	2.20	0.45
1:L:139:PHE:HB2	1:L:140:TYR:H	1.36	0.45
1:L:184:GLU:O	1:L:188:HIS:HD2	1.92	0.45
2:H:93:MET:CE	2:H:113:GLY:C	2.84	0.45
2:H:130:PRO:O	2:H:131:LEU:HD23	2.17	0.45
2:H:29:PHE:CE2	2:H:72:ARG:HD3	2.51	0.45
3:A:12:ILE:CD1	3:A:17:LEU:HD23	2.38	0.45
1:L:83:LEU:O	1:L:84:ALA:HB2	2.17	0.45
2:H:161:TRP:CZ3	2:H:217:ILE:CD1	3.00	0.45
2:H:5:VAL:O	2:H:5:VAL:CG2	2.65	0.45
2:H:201:THR:HG22	2:H:214:ASP:HB3	1.99	0.45
2:H:86:LEU:HA	2:H:86:LEU:HD23	1.67	0.45
1:L:41:GLU:HG3	4:L:348:HOH:O	2.16	0.44
3:A:28:ALA:O	3:A:57:PHE:CZ	2.68	0.44
1:L:193:CYS:HB3	1:L:206:LYS:CB	2.46	0.44
1:L:180:LEU:HD12	1:L:185:TYR:CB	2.38	0.44
3:A:13:ASN:O	3:A:60:THR:HA	2.18	0.44
2:H:51:ILE:HG13	2:H:70:ILE:HD13	2.00	0.44
2:H:166:LEU:CB	4:H:329:HOH:O	2.34	0.44
1:L:108:ARG:CG	1:L:108:ARG:NH1	2.81	0.44
2:H:171:HIS:O	2:H:186:SER:HA	2.18	0.44
1:L:139:PHE:CZ	1:L:174:MET:HB2	2.47	0.44
2:H:35:HIS:CD2	2:H:47:TRP:NE1	2.83	0.44
2:H:122:LYS:HE2	2:H:122:LYS:HA	2.00	0.44
1:L:61:ARG:NH2	1:L:82:ASP:OD1	2.35	0.44
1:L:108:ARG:HG2	1:L:109:ALA:H	1.83	0.44
1:L:7:SER:HB2	4:L:354:HOH:O	2.16	0.44
1:L:12:SER:HA	1:L:105:GLU:O	2.17	0.44
1:L:156:ASN:C	1:L:156:ASN:ND2	2.70	0.44
1:L:30:VAL:HG22	1:L:31:THR:N	2.29	0.44
1:L:150:ILE:HB	1:L:153:GLU:O	2.18	0.43
2:H:62:ASP:HA	2:H:65:LYS:CE	2.39	0.43
2:H:171:HIS:CD2	4:H:231:HOH:O	2.71	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:155:GLN:HB3	1:L:156:ASN:H	1.35	0.43
2:H:93:MET:HE3	2:H:114:THR:N	2.33	0.43
1:L:159:LEU:HA	1:L:159:LEU:HD23	1.86	0.43
1:L:208:PHE:CD1	1:L:208:PHE:O	2.72	0.43
1:L:123:GLU:OE1	1:L:123:GLU:N	2.40	0.43
1:L:147:LYS:HD2	1:L:194:GLU:O	2.19	0.43
1:L:24:LYS:HB2	1:L:24:LYS:HE3	1.72	0.43
3:A:7:THR:OG1	3:A:24:LYS:NZ	2.44	0.43
1:L:169:ASP:OD1	1:L:169:ASP:O	2.37	0.43
3:A:32:GLU:HG3	4:A:86:HOH:O	2.18	0.43
1:L:117:ILE:CD1	1:L:148:TRP:HZ3	2.32	0.43
1:L:17:GLU:O	1:L:78:VAL:HG23	2.19	0.42
1:L:4:MET:HE2	1:L:90:GLN:HB3	2.01	0.42
1:L:180:LEU:HG	1:L:180:LEU:H	1.66	0.42
2:H:126:PRO:HB2	2:H:149:VAL:HG13	2.00	0.42
1:L:88:CYS:O	1:L:98:PHE:HA	2.20	0.42
2:H:157:VAL:HA	2:H:205:ALA:O	2.20	0.42
1:L:197:HIS:O	1:L:199:THR:N	2.51	0.42
1:L:139:PHE:HE2	1:L:162:TRP:CZ3	2.38	0.42
1:L:110:ASP:OD1	1:L:198:LYS:NZ	2.46	0.42
2:H:45:LEU:H	2:H:45:LEU:HG	1.44	0.42
1:L:118:PHE:HA	1:L:119:PRO:HD3	1.72	0.42
1:L:183:ASP:O	1:L:187:ARG:NH2	2.53	0.42
1:L:132:VAL:CG1	1:L:208:PHE:HE2	2.33	0.42
1:L:90:GLN:HE21	1:L:90:GLN:HB2	1.33	0.42
2:H:124:THR:HG21	2:H:181:LEU:HD22	2.02	0.42
2:H:87:ARG:HD3	2:H:87:ARG:HA	1.84	0.42
2:H:150:LYS:HG3	2:H:151:GLY:N	2.35	0.42
2:H:164:GLY:C	2:H:166:LEU:H	2.22	0.42
1:L:121:SER:HB3	1:L:123:GLU:OE1	2.20	0.42
2:H:124:THR:HG21	2:H:181:LEU:CD2	2.50	0.42
2:H:68:PHE:CZ	2:H:83:MET:HE2	2.55	0.42
1:L:182:LYS:O	1:L:186:GLU:HG2	2.19	0.41
3:A:39:ALA:O	3:A:44:VAL:N	2.41	0.41
1:L:110:ASP:CG	1:L:198:LYS:HE3	2.40	0.41
2:H:72:ARG:HD3	2:H:74:ASN:OD1	2.20	0.41
2:H:4:LEU:HD12	2:H:24:ALA:HA	2.01	0.41
2:H:210:SER:HA	4:H:364:HOH:O	2.19	0.41
1:L:117:ILE:CD1	1:L:148:TRP:CZ3	3.03	0.41
1:L:196:THR:HG22	1:L:200:SER:O	2.20	0.41
1:L:178:LEU:HG	1:L:180:LEU:HD21	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:183:ASP:N	1:L:183:ASP:OD1	2.53	0.41
1:L:13:MET:HB3	1:L:13:MET:HE2	1.86	0.41
1:L:71:PHE:N	1:L:71:PHE:CD1	2.89	0.41
2:H:127:SER:HA	3:A:42:ASN:ND2	2.34	0.41
1:L:190:SER:HA	1:L:209:ASN:HA	2.02	0.41
2:H:159:VAL:HA	2:H:203:ASN:O	2.20	0.41
1:L:59:PRO:O	1:L:61:ARG:N	2.53	0.41
1:L:28:ASN:CG	1:L:68:ALA:HB1	2.40	0.41
3:A:59:VAL:CG1	3:A:59:VAL:O	2.69	0.41
3:A:12:ILE:HB	3:A:59:VAL:CG1	2.42	0.41
2:H:38:ARG:CG	2:H:48:VAL:HG21	2.44	0.41
2:H:85:SER:O	2:H:86:LEU:C	2.59	0.41
2:H:180:ASP:O	2:H:181:LEU:CG	2.66	0.41
1:L:13:MET:CG	1:L:19:VAL:CG2	2.93	0.41
1:L:112:ALA:HA	1:L:113:PRO:HD3	1.84	0.41
1:L:146:VAL:HG13	1:L:146:VAL:O	2.21	0.41
1:L:136:LEU:O	1:L:139:PHE:HE1	2.04	0.41
1:L:182:LYS:HB3	1:L:182:LYS:HZ2	1.85	0.40
1:L:182:LYS:C	1:L:186:GLU:HG3	2.42	0.40
1:L:79:GLN:CG	1:L:80:ALA:H	2.32	0.40
2:H:157:VAL:HG22	2:H:184:LEU:CD2	2.47	0.40
1:L:45:LYS:N	1:L:45:LYS:HD2	2.35	0.40
2:H:133:PRO:HB3	2:H:138:GLN:HE21	1.86	0.40
2:H:122:LYS:NZ	2:H:123:THR:HG23	2.35	0.40
1:L:33:VAL:HG21	1:L:71:PHE:CD1	2.56	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	L	211/213 (99%)	177 (84%)	18 (8%)	16 (8%)	1 1

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	H	220/222 (99%)	183 (83%)	23 (10%)	14 (6%)	2 2
3	A	56/61 (92%)	53 (95%)	2 (4%)	1 (2%)	11 21
All	All	487/496 (98%)	413 (85%)	43 (9%)	31 (6%)	2 2

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	60	ASP
1	L	82	ASP
1	L	140	TYR
1	L	141	PRO
1	L	150	ILE
1	L	170	SER
1	L	198	LYS
1	L	207	SER
1	L	208	PHE
2	H	30	SER
2	H	43	LYS
2	H	85	SER
2	H	141	SER
2	H	168	SER
2	H	196	PRO
2	H	221	ASP
3	A	6	THR
1	L	9	LYS
1	L	41	GLU
1	L	152	SER
1	L	184	GLU
2	H	29	PHE
2	H	137	ALA
2	H	193	SER
1	L	187	ARG
2	H	99	TRP
2	H	134	GLY
2	H	136	ALA
1	L	30	VAL
1	L	210	ARG
2	H	77	ASN

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	L	190/190 (100%)	141 (74%)	49 (26%)	0 1
2	H	189/189 (100%)	143 (76%)	46 (24%)	1 1
3	A	47/50 (94%)	39 (83%)	8 (17%)	2 4
All	All	426/429 (99%)	323 (76%)	103 (24%)	1 1

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASN
1	L	10	SER
1	L	12	SER
1	L	14	SER
1	L	17	GLU
1	L	19	VAL
1	L	24	LYS
1	L	41	GLU
1	L	45	LYS
1	L	67	SER
1	L	72	THR
1	L	75	ILE
1	L	77	SER
1	L	81	GLU
1	L	82	ASP
1	L	85	ASP
1	L	90	GLN
1	L	93	SER
1	L	103	LYS
1	L	108	ARG
1	L	122	SER
1	L	136	LEU
1	L	139	PHE
1	L	142	LYS
1	L	144	ILE
1	L	147	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	153	GLU
1	L	156	ASN
1	L	161	SER
1	L	168	LYS
1	L	174	MET
1	L	175	SER
1	L	176	SER
1	L	178	LEU
1	L	180	LEU
1	L	181	THR
1	L	182	LYS
1	L	183	ASP
1	L	187	ARG
1	L	192	THR
1	L	196	THR
1	L	198	LYS
1	L	201	THR
1	L	206	LYS
1	L	208	PHE
1	L	209	ASN
1	L	211	ASN
1	L	212	GLU
1	L	213	CYS
2	H	1	ASP
2	H	3	GLN
2	H	4	LEU
2	H	6	GLU
2	H	7	SER
2	H	13	GLN
2	H	17	SER
2	H	22	CYS
2	H	38	ARG
2	H	51	ILE
2	H	53	SER
2	H	55	SER
2	H	58	LEU
2	H	64	VAL
2	H	72	ARG
2	H	78	THR
2	H	82	GLN
2	H	87	ARG
2	H	107	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	108	ASP
2	H	112	GLN
2	H	122	LYS
2	H	123	THR
2	H	126	PRO
2	H	139	THR
2	H	144	THR
2	H	145	LEU
2	H	148	LEU
2	H	165	SER
2	H	167	SER
2	H	176	VAL
2	H	178	GLN
2	H	180	ASP
2	H	183	THR
2	H	185	SER
2	H	188	VAL
2	H	189	THR
2	H	190	VAL
2	H	192	SER
2	H	193	SER
2	H	198	GLU
2	H	213	VAL
2	H	214	ASP
2	H	220	ARG
2	H	221	ASP
2	H	222	CYS
3	A	12	ILE
3	A	20	GLU
3	A	21	THR
3	A	23	THR
3	A	26	VAL
3	A	33	LYS
3	A	55	LYS
3	A	60	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	38	GLN
1	L	90	GLN
1	L	155	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	156	ASN
1	L	160	ASN
1	L	188	HIS
2	H	13	GLN
2	H	35	HIS
2	H	39	GLN
2	H	82	GLN
2	H	112	GLN
2	H	178	GLN
2	H	203	ASN
3	A	40	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	L	213/213 (100%)	-0.94	2 (0%) 85 83	9, 28, 59, 118	0
2	H	222/222 (100%)	-0.95	2 (0%) 85 83	9, 24, 62, 104	0
3	A	58/61 (95%)	-1.02	0 100 100	14, 30, 45, 71	0
All	All	493/496 (99%)	-0.96	4 (0%) 87 85	9, 26, 60, 118	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	212	GLU	6.7
1	L	213	CYS	5.8
2	H	221	ASP	2.8
2	H	134	GLY	2.7

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.