Full wwPDB X-ray Structure Validation Report (i)

PDB ID	:	3EYQ
Title	:	Crystal structure of MJ5 Fab, a germline antibody variant of anti-human cytomegalovirus antibody 8f9
Authors	:	Thomson, C.A.; Bryson, S.; McLean, G.R.; Creagh, A.L.; Pai, E.F.; Schrader, J.W.
Deposited on	:	2008-10-21
Resolution	:	2.40 Å(reported)

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

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

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Clashscore		26
Ramachandran outliers		4.6%
Sidechain outliers		23.1%
RSRZ outliers		0.5%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
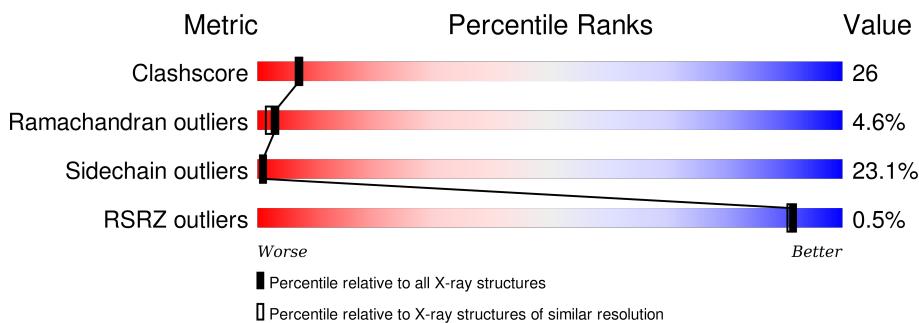
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	C	216	32% 36% 24% 6% ·
2	D	242	% 35% 32% 16% · 14%
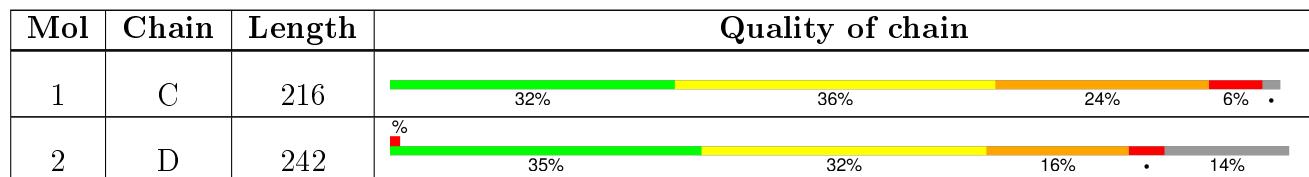
2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 3294 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 M2J5 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	212	Total 1638	C 1026	N 280	O 328	S 4	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	EXPRESSION TAG	PDB 3EYQ

- Molecule 2 is a protein called 8f9 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	208	Total 1568	C 994	N 264	O 304	S 6	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	235	LEU	-	EXPRESSION TAG	PDB 3EYQ
D	236	GLU	-	EXPRESSION TAG	PDB 3EYQ
D	237	HIS	-	EXPRESSION TAG	PDB 3EYQ
D	238	HIS	-	EXPRESSION TAG	PDB 3EYQ
D	239	HIS	-	EXPRESSION TAG	PDB 3EYQ
D	240	HIS	-	EXPRESSION TAG	PDB 3EYQ
D	241	HIS	-	EXPRESSION TAG	PDB 3EYQ
D	242	HIS	-	EXPRESSION TAG	PDB 3EYQ

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	55	Total 55	O 55	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	33	Total 33	O 33	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: M2J5 Fab

Chain C:

- Molecule 2: 8f9 Fab

Chain D:
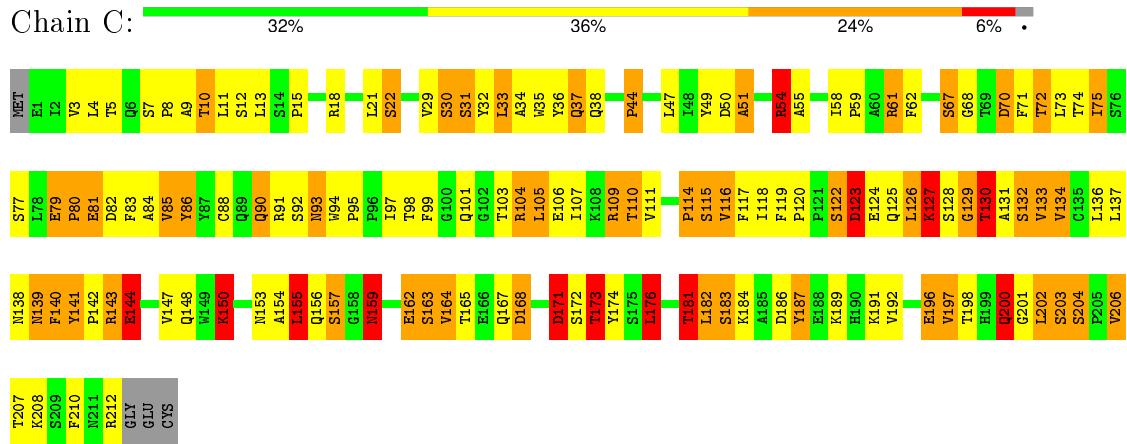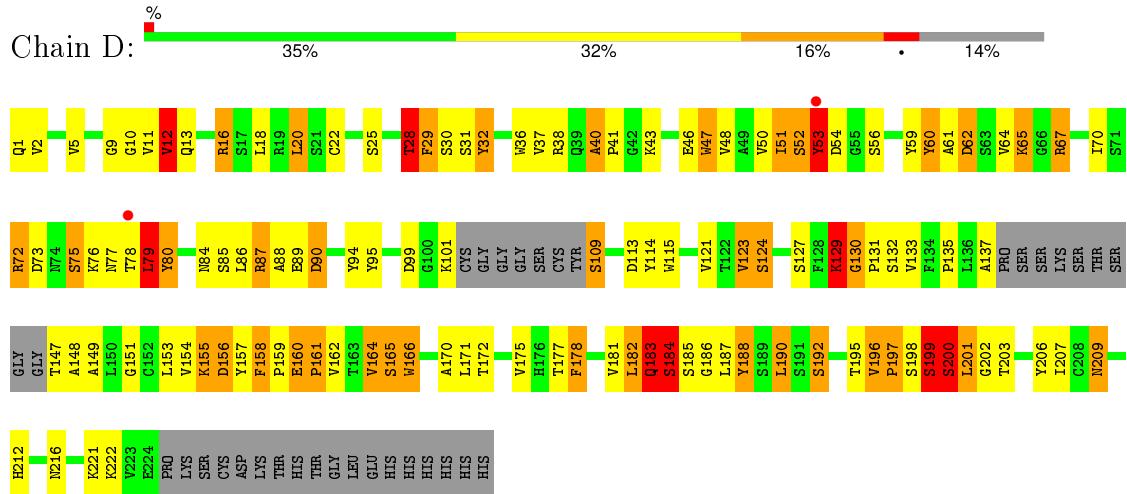
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	65.38Å　　76.05Å　　111.54Å 90.00°　　90.00°　　90.00°	Depositor
Resolution (Å)	50.00　–　2.40 56.40　–　2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.40) 85.9 (56.40-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.75 (at 2.40Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.250　,　　　0.270 0.262　,　(Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	22.1	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 49.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.46$, $<L^2> = 0.29$	Xtriage
Outliers	0 of 20540 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	3294	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	C	2.52	76/1675 (4.5%)	1.57	21/2279 (0.9%)
2	D	2.42	62/1603 (3.9%)	1.49	15/2177 (0.7%)
All	All	2.47	138/3278 (4.2%)	1.53	36/4456 (0.8%)

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	C	4	8
2	D	4	14
All	All	8	22

All (138) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	174	TYR	CE1-CZ	-11.03	1.24	1.38
1	C	32	TYR	CD1-CE1	-11.03	1.22	1.39
1	C	32	TYR	CD2-CE2	-10.86	1.23	1.39
1	C	174	TYR	CD2-CE2	-10.23	1.24	1.39
1	C	134	VAL	CB-CG2	-10.18	1.31	1.52
1	C	174	TYR	CD1-CE1	-9.99	1.24	1.39
1	C	206	VAL	CB-CG1	-9.96	1.31	1.52
2	D	11	VAL	CB-CG2	-9.89	1.32	1.52
1	C	164	VAL	CB-CG2	-9.18	1.33	1.52
2	D	155	LYS	CE-NZ	-9.16	1.26	1.49
1	C	134	VAL	CB-CG1	-9.12	1.33	1.52
1	C	49	TYR	CD1-CE1	-8.78	1.26	1.39
2	D	157	TYR	CD1-CE1	-8.78	1.26	1.39
2	D	158	PHE	CD1-CE1	-8.75	1.21	1.39
2	D	188	TYR	CD1-CE1	-8.66	1.26	1.39
2	D	123	VAL	CB-CG1	-8.40	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	36	TYR	CD1-CE1	-8.36	1.26	1.39
2	D	166	TRP	CE3-CZ3	-8.10	1.24	1.38
2	D	115	TRP	CE3-CZ3	-8.06	1.24	1.38
1	C	36	TYR	CD2-CE2	-8.04	1.27	1.39
2	D	188	TYR	CD2-CE2	-8.02	1.27	1.39
1	C	192	VAL	CB-CG2	-7.88	1.36	1.52
1	C	171	ASP	CB-CG	-7.85	1.35	1.51
2	D	121	VAL	CB-CG2	-7.79	1.36	1.52
2	D	158	PHE	CD2-CE2	-7.77	1.23	1.39
1	C	119	PHE	CD1-CE1	-7.74	1.23	1.39
2	D	154	VAL	CB-CG1	-7.73	1.36	1.52
2	D	48	VAL	CB-CG1	-7.64	1.36	1.52
2	D	157	TYR	CD2-CE2	-7.63	1.27	1.39
1	C	86	TYR	CD1-CE1	-7.59	1.27	1.39
2	D	114	TYR	CD2-CE2	-7.57	1.27	1.39
2	D	61	ALA	CA-CB	-7.44	1.36	1.52
1	C	196	GLU	CD-OE1	-7.41	1.17	1.25
2	D	137	ALA	CA-CB	-7.34	1.37	1.52
1	C	164	VAL	CB-CG1	-7.25	1.37	1.52
1	C	127	LYS	CB-CG	-7.22	1.33	1.52
2	D	154	VAL	CB-CG2	-7.20	1.37	1.52
1	C	119	PHE	CD2-CE2	-7.07	1.25	1.39
1	C	197	VAL	CB-CG1	-7.07	1.38	1.52
2	D	164	VAL	CB-CG2	-7.06	1.38	1.52
1	C	67	SER	CB-OG	-7.03	1.33	1.42
1	C	140	PHE	CD1-CE1	-7.03	1.25	1.39
1	C	140	PHE	CD2-CE2	-6.98	1.25	1.39
2	D	12	VAL	CB-CG1	-6.97	1.38	1.52
2	D	40	ALA	CA-CB	-6.91	1.38	1.52
2	D	170	ALA	CA-CB	-6.88	1.38	1.52
1	C	86	TYR	CD2-CE2	-6.82	1.29	1.39
2	D	196	VAL	CB-CG1	-6.79	1.38	1.52
1	C	85	VAL	CB-CG2	-6.76	1.38	1.52
2	D	11	VAL	CB-CG1	-6.71	1.38	1.52
1	C	70	ASP	CB-CG	-6.71	1.37	1.51
1	C	198	THR	CB-CG2	-6.65	1.30	1.52
2	D	59	TYR	CD1-CE1	-6.59	1.29	1.39
2	D	178	PHE	CD2-CE2	-6.55	1.26	1.39
2	D	114	TYR	CE2-CZ	-6.52	1.30	1.38
1	C	154	ALA	CA-CB	-6.51	1.38	1.52
1	C	85	VAL	CB-CG1	-6.48	1.39	1.52
2	D	148	ALA	CA-CB	-6.48	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	5	VAL	CB-CG1	-6.48	1.39	1.52
2	D	147	THR	CB-CG2	-6.44	1.31	1.52
1	C	71	PHE	CE2-CZ	-6.26	1.25	1.37
2	D	188	TYR	CE1-CZ	-6.16	1.30	1.38
2	D	184	SER	CB-OG	-6.11	1.34	1.42
2	D	114	TYR	CD1-CE1	-6.11	1.30	1.39
2	D	206	TYR	CE1-CZ	-6.08	1.30	1.38
1	C	133	VAL	CB-CG2	-6.04	1.40	1.52
2	D	175	VAL	CB-CG2	-6.01	1.40	1.52
1	C	162	GLU	CD-OE1	-6.01	1.19	1.25
2	D	46	GLU	CD-OE1	-6.00	1.19	1.25
2	D	32	TYR	CD1-CE1	-5.98	1.30	1.39
1	C	143	ARG	CB-CG	-5.92	1.36	1.52
1	C	174	TYR	CG-CD2	-5.92	1.31	1.39
1	C	49	TYR	CD2-CE2	-5.87	1.30	1.39
1	C	37	GLN	C-O	-5.86	1.12	1.23
2	D	178	PHE	CD1-CE1	-5.84	1.27	1.39
1	C	187	TYR	CD1-CE1	-5.82	1.30	1.39
1	C	116	VAL	CB-CG2	-5.81	1.40	1.52
2	D	95	TYR	CE1-CZ	-5.80	1.31	1.38
1	C	174	TYR	CZ-OH	-5.79	1.28	1.37
1	C	163	SER	CB-OG	-5.79	1.34	1.42
1	C	10	THR	CB-CG2	-5.77	1.33	1.52
1	C	122	SER	CB-OG	-5.73	1.34	1.42
2	D	32	TYR	CD2-CE2	-5.73	1.30	1.39
1	C	120	PRO	CB-CG	-5.72	1.21	1.50
2	D	37	VAL	CA-CB	5.68	1.66	1.54
1	C	71	PHE	CD2-CE2	-5.67	1.27	1.39
2	D	197	PRO	CG-CD	-5.67	1.31	1.50
1	C	150	LYS	CB-CG	-5.65	1.37	1.52
1	C	181	THR	CB-CG2	-5.61	1.33	1.52
2	D	129	LYS	CG-CD	-5.61	1.33	1.52
1	C	144	GLU	CD-OE1	-5.60	1.19	1.25
1	C	196	GLU	CD-OE2	-5.59	1.19	1.25
1	C	9	ALA	CA-CB	-5.57	1.40	1.52
2	D	2	VAL	CB-CG1	-5.57	1.41	1.52
2	D	114	TYR	CG-CD2	-5.56	1.31	1.39
1	C	147	VAL	CB-CG2	-5.54	1.41	1.52
1	C	140	PHE	CE2-CZ	-5.54	1.26	1.37
1	C	141	TYR	CE2-CZ	-5.54	1.31	1.38
2	D	94	TYR	CE1-CZ	-5.53	1.31	1.38
2	D	80	TYR	CD2-CE2	-5.52	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	33	LEU	C-O	-5.52	1.12	1.23
2	D	206	TYR	CD1-CE1	-5.51	1.31	1.39
2	D	38	ARG	CG-CD	-5.50	1.38	1.51
2	D	130	GLY	C-O	-5.47	1.14	1.23
1	C	22	SER	CB-OG	-5.45	1.35	1.42
1	C	118	ILE	CB-CG2	-5.44	1.35	1.52
2	D	32	TYR	CE2-CZ	-5.44	1.31	1.38
1	C	118	ILE	C-O	-5.43	1.13	1.23
2	D	60	TYR	CD2-CE2	-5.42	1.31	1.39
2	D	206	TYR	CD2-CE2	-5.42	1.31	1.39
2	D	160	GLU	CD-OE2	-5.41	1.19	1.25
1	C	201	GLY	C-O	-5.40	1.15	1.23
1	C	86	TYR	CB-CG	-5.36	1.43	1.51
1	C	119	PHE	CG-CD1	-5.35	1.30	1.38
1	C	210	PHE	CD1-CE1	-5.35	1.28	1.39
2	D	133	VAL	CB-CG2	-5.33	1.41	1.52
1	C	71	PHE	CE1-CZ	-5.33	1.27	1.37
1	C	132	SER	CB-OG	-5.31	1.35	1.42
1	C	84	ALA	CA-CB	-5.30	1.41	1.52
1	C	109	ARG	CZ-NH1	-5.29	1.26	1.33
1	C	82	ASP	CB-CG	-5.28	1.40	1.51
1	C	155	LEU	N-CA	-5.20	1.35	1.46
1	C	157	SER	CB-OG	-5.15	1.35	1.42
2	D	47	TRP	CE3-CZ3	-5.15	1.29	1.38
1	C	30	SER	CB-OG	-5.13	1.35	1.42
1	C	110	THR	N-CA	-5.12	1.36	1.46
2	D	95	TYR	CD1-CE1	-5.09	1.31	1.39
1	C	173	THR	C-O	-5.08	1.13	1.23
2	D	32	TYR	CG-CD1	-5.07	1.32	1.39
1	C	68	GLY	C-O	-5.07	1.15	1.23
2	D	64	VAL	CB-CG1	-5.07	1.42	1.52
2	D	114	TYR	C-O	-5.05	1.13	1.23
1	C	111	VAL	CB-CG2	-5.04	1.42	1.52
1	C	79	GLU	CD-OE1	-5.04	1.20	1.25
1	C	3	VAL	CB-CG1	-5.03	1.42	1.52
1	C	204	SER	CB-OG	-5.02	1.35	1.42
2	D	115	TRP	CG-CD1	-5.00	1.29	1.36
2	D	186	GLY	C-O	-5.00	1.15	1.23

All (36) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	123	ASP	CB-CG-OD2	9.79	127.12	118.30
1	C	186	ASP	CB-CG-OD2	9.52	126.87	118.30
2	D	73	ASP	CB-CG-OD2	8.32	125.79	118.30
1	C	168	ASP	CB-CG-OD2	8.11	125.60	118.30
1	C	176	LEU	CA-CB-CG	7.47	132.48	115.30
2	D	53	TYR	CA-CB-CG	7.25	127.17	113.40
1	C	61	ARG	NE-CZ-NH1	7.09	123.85	120.30
2	D	62	ASP	CB-CG-OD2	6.99	124.59	118.30
1	C	51	ALA	N-CA-C	6.49	128.52	111.00
2	D	28	THR	N-CA-C	6.48	128.51	111.00
2	D	67	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	C	130	THR	N-CA-C	6.21	127.76	111.00
2	D	53	TYR	CB-CG-CD2	6.18	124.71	121.00
2	D	171	LEU	CA-CB-CG	6.07	129.27	115.30
2	D	190	LEU	CA-CB-CG	6.04	129.20	115.30
2	D	20	LEU	CA-CB-CG	6.03	129.17	115.30
2	D	79	LEU	CA-CB-CG	5.99	129.07	115.30
1	C	72	THR	OG1-CB-CG2	-5.96	96.30	110.00
1	C	176	LEU	CB-CG-CD1	5.95	121.12	111.00
1	C	70	ASP	CB-CG-OD2	5.95	123.65	118.30
1	C	212	ARG	NE-CZ-NH1	5.88	123.24	120.30
2	D	99	ASP	CB-CG-OD1	5.84	123.56	118.30
2	D	90	ASP	CB-CG-OD2	5.81	123.53	118.30
1	C	201	GLY	N-CA-C	5.66	127.26	113.10
1	C	115	SER	N-CA-C	5.61	126.14	111.00
2	D	113	ASP	N-CA-C	5.60	126.12	111.00
1	C	50	ASP	CB-CG-OD1	5.38	123.14	118.30
1	C	5	THR	OG1-CB-CG2	-5.30	97.81	110.00
1	C	120	PRO	N-CD-CG	-5.29	95.27	103.20
1	C	134	VAL	CB-CA-C	5.22	121.32	111.40
2	D	184	SER	N-CA-C	5.20	125.04	111.00
1	C	10	THR	N-CA-C	5.20	125.03	111.00
1	C	159	ASN	N-CA-C	5.19	125.02	111.00
1	C	200	GLN	N-CA-C	5.14	124.87	111.00
1	C	171	ASP	CB-CG-OD1	5.08	122.87	118.30
2	D	153	LEU	CB-CG-CD2	5.05	119.59	111.00

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	51	ALA	CA

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Mol	Chain	Res	Type	Atom
1	C	115	SER	CA
1	C	123	ASP	CA
1	C	130	THR	CA
2	D	28	THR	CA
2	D	113	ASP	CA
2	D	147	THR	CA
2	D	183	GLN	CA

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	114	PRO	Peptide
1	C	122	SER	Peptide
1	C	129	GLY	Peptide
1	C	181	THR	Peptide
1	C	51	ALA	Peptide
1	C	54	ARG	Peptide
1	C	80	PRO	Peptide
1	C	99	PHE	Peptide
2	D	10	GLY	Peptide
2	D	131	PRO	Peptide
2	D	155	LYS	Peptide
2	D	181	VAL	Peptide
2	D	182	LEU	Peptide
2	D	184	SER	Peptide
2	D	198	SER	Peptide
2	D	199	SER	Peptide
2	D	202	GLY	Peptide
2	D	29	PHE	Peptide
2	D	52	SER	Peptide
2	D	53	TYR	Peptide
2	D	75	SER	Peptide
2	D	9	GLY	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	C	1638	0	1597	97	0
2	D	1568	0	1539	71	5
3	C	55	0	0	5	0
3	D	33	0	0	2	0
All	All	3294	0	3136	166	5

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 26.

All (166) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:ASP:HB3	1:C:173:THR:OG1	1.50	1.11
1:C:130:THR:HG22	1:C:131:ALA:H	0.94	1.05
1:C:127:LYS:HD2	1:C:127:LYS:N	1.73	1.03
1:C:130:THR:HG22	1:C:131:ALA:N	1.74	0.99
2:D:67:ARG:NH2	2:D:90:ASP:OD2	1.96	0.96
1:C:130:THR:CG2	1:C:131:ALA:H	1.81	0.94
1:C:126:LEU:O	1:C:184:LYS:HD2	1.72	0.89
1:C:12:SER:OG	1:C:106:GLU:OE2	1.91	0.87
2:D:53:TYR:HB3	2:D:54:ASP:CB	2.05	0.87
2:D:36:TRP:NE1	2:D:79:LEU:HD11	1.91	0.86
2:D:36:TRP:CE2	2:D:79:LEU:HD11	2.11	0.85
1:C:127:LYS:C	1:C:129:GLY:H	1.81	0.81
1:C:29:VAL:O	1:C:29:VAL:HG22	1.79	0.80
2:D:87:ARG:CD	2:D:89:GLU:OE2	2.30	0.80
1:C:37:GLN:HB2	1:C:47:LEU:HD11	1.64	0.79
2:D:177:THR:OG1	2:D:192:SER:OG	1.94	0.79
2:D:36:TRP:CE2	2:D:79:LEU:CD1	2.64	0.79
1:C:127:LYS:N	1:C:127:LYS:CD	2.30	0.79
1:C:126:LEU:O	1:C:184:LYS:CD	2.31	0.78
2:D:200:SER:O	2:D:201:LEU:HB2	1.83	0.78
1:C:29:VAL:HG23	1:C:92:SER:HB2	1.64	0.78
1:C:171:ASP:CB	1:C:173:THR:OG1	2.30	0.77
2:D:87:ARG:HD3	2:D:89:GLU:OE2	1.85	0.77
2:D:36:TRP:CZ2	2:D:79:LEU:HD13	2.22	0.75
2:D:12:VAL:HG11	2:D:86:LEU:HD13	1.68	0.75
2:D:53:TYR:HB3	2:D:54:ASP:HB2	1.68	0.75
2:D:200:SER:O	2:D:201:LEU:CB	2.35	0.74
1:C:104:ARG:NH2	3:C:252:HOH:O	2.20	0.73
1:C:29:VAL:O	1:C:29:VAL:CG2	2.36	0.73
2:D:12:VAL:HG12	2:D:123:VAL:HG22	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:28:THR:C	2:D:30:SER:H	1.89	0.73
1:C:156:GLN:HB3	1:C:159:ASN:HD21	1.52	0.72
1:C:107:ILE:H	1:C:167:GLN:HE22	1.38	0.72
2:D:54:ASP:OD2	2:D:56:SER:HB2	1.90	0.72
2:D:67:ARG:HB3	2:D:84:ASN:O	1.91	0.71
2:D:67:ARG:HH22	2:D:90:ASP:CG	1.93	0.71
2:D:36:TRP:CZ2	2:D:79:LEU:CD1	2.74	0.70
2:D:199:SER:C	2:D:200:SER:O	2.28	0.70
1:C:15:PRO:HD3	1:C:83:PHE:CZ	2.26	0.70
1:C:127:LYS:C	1:C:129:GLY:N	2.44	0.69
2:D:36:TRP:NE1	2:D:79:LEU:CD1	2.56	0.67
2:D:87:ARG:HD2	2:D:89:GLU:OE2	1.93	0.67
2:D:29:PHE:O	2:D:72:ARG:NH2	2.27	0.66
2:D:13:GLN:OE1	2:D:16:ARG:NH2	2.29	0.66
2:D:129:LYS:HG3	2:D:130:GLY:N	2.11	0.65
1:C:30:SER:OG	1:C:31:SER:N	2.30	0.65
1:C:125:GLN:O	1:C:127:LYS:N	2.30	0.65
2:D:28:THR:O	2:D:30:SER:N	2.30	0.65
2:D:53:TYR:HB3	2:D:54:ASP:HB3	1.79	0.64
1:C:21:LEU:HB2	1:C:73:LEU:HB3	1.81	0.63
1:C:29:VAL:HG23	1:C:92:SER:CB	2.29	0.63
1:C:123:ASP:O	1:C:127:LYS:HD3	2.00	0.62
2:D:196:VAL:HB	2:D:197:PRO:HD2	1.81	0.62
2:D:196:VAL:HB	2:D:197:PRO:CD	2.29	0.62
1:C:202:LEU:O	1:C:203:SER:C	2.35	0.62
2:D:54:ASP:OD2	2:D:56:SER:CB	2.47	0.62
1:C:38:GLN:NE2	1:C:44:PRO:HD3	2.16	0.60
1:C:83:PHE:CE1	1:C:107:ILE:HG13	2.35	0.60
1:C:38:GLN:HE21	1:C:44:PRO:HD3	1.66	0.60
1:C:130:THR:CG2	1:C:131:ALA:N	2.49	0.60
1:C:104:ARG:NH1	3:C:263:HOH:O	2.35	0.59
1:C:116:VAL:HG12	1:C:208:LYS:HG2	1.83	0.59
1:C:116:VAL:HG12	1:C:208:LYS:CG	2.32	0.59
1:C:90:GLN:OE1	1:C:98:THR:OG1	2.21	0.58
2:D:52:SER:O	2:D:54:ASP:N	2.37	0.58
1:C:117:PHE:HB2	1:C:136:LEU:HB3	1.84	0.58
1:C:85:VAL:HG22	1:C:104:ARG:HB2	1.85	0.57
1:C:150:LYS:HG2	1:C:153:ASN:HA	1.85	0.57
2:D:53:TYR:CG	2:D:54:ASP:HB2	2.40	0.57
2:D:60:TYR:CE1	2:D:70:ILE:HG22	2.39	0.57
1:C:126:LEU:C	1:C:127:LYS:HD2	2.26	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:PRO:HD3	1:C:83:PHE:HZ	1.68	0.56
2:D:199:SER:OG	2:D:200:SER:N	2.28	0.55
1:C:144:GLU:CD	1:C:144:GLU:H	2.10	0.55
2:D:62:ASP:HA	2:D:65:LYS:HD2	1.89	0.55
1:C:83:PHE:CD1	1:C:107:ILE:HG13	2.43	0.54
1:C:124:GLU:HG3	1:C:124:GLU:O	2.06	0.54
1:C:35:TRP:CE3	1:C:73:LEU:HD22	2.42	0.54
2:D:52:SER:O	2:D:53:TYR:C	2.45	0.54
2:D:47:TRP:HZ2	2:D:50:VAL:HG12	1.73	0.53
1:C:197:VAL:HB	1:C:206:VAL:HG23	1.91	0.53
2:D:53:TYR:CB	2:D:54:ASP:HB2	2.36	0.53
1:C:37:GLN:HG3	1:C:86:TYR:CE1	2.44	0.52
1:C:11:LEU:HB3	1:C:105:LEU:HG	1.92	0.52
1:C:197:VAL:HB	1:C:206:VAL:CG2	2.40	0.52
1:C:168:ASP:HB3	1:C:173:THR:H	1.74	0.52
1:C:125:GLN:NE2	1:C:132:SER:H	2.08	0.51
2:D:52:SER:C	2:D:54:ASP:N	2.63	0.51
1:C:61:ARG:O	1:C:75:ILE:HA	2.10	0.51
1:C:125:GLN:HE22	1:C:132:SER:H	1.57	0.51
2:D:22:CYS:HB3	2:D:79:LEU:HD12	1.93	0.51
2:D:22:CYS:N	2:D:79:LEU:O	2.43	0.51
2:D:36:TRP:CE2	2:D:79:LEU:HD13	2.43	0.51
2:D:29:PHE:HB3	2:D:77:ASN:OD1	2.11	0.50
1:C:182:LEU:HD13	1:C:187:TYR:HB2	1.94	0.50
1:C:124:GLU:O	1:C:127:LYS:HG2	2.11	0.50
2:D:129:LYS:O	2:D:212:HIS:CE1	2.64	0.50
1:C:141:TYR:CG	1:C:142:PRO:HA	2.46	0.50
1:C:144:GLU:O	3:C:251:HOH:O	2.20	0.49
1:C:55:ALA:HB3	1:C:58:ILE:HG13	1.95	0.49
1:C:35:TRP:CE2	1:C:73:LEU:HB2	2.48	0.49
2:D:129:LYS:O	2:D:212:HIS:HE1	1.96	0.48
2:D:51:ILE:HB	2:D:70:ILE:HG12	1.93	0.48
2:D:135:PRO:HD3	2:D:221:LYS:HE2	1.96	0.48
2:D:40:ALA:HB1	2:D:41:PRO:HD2	1.95	0.48
2:D:54:ASP:OD2	2:D:56:SER:OG	2.30	0.48
2:D:165:SER:HB3	2:D:209:ASN:OD1	2.14	0.48
1:C:94:TRP:HB2	1:C:95:PRO:HA	1.96	0.48
1:C:168:ASP:CG	1:C:171:ASP:HB2	2.35	0.47
1:C:90:GLN:NE2	1:C:93:ASN:O	2.47	0.47
2:D:151:GLY:HA2	2:D:166:TRP:CH2	2.48	0.47
1:C:168:ASP:O	1:C:172:SER:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:PHE:CE1	1:C:75:ILE:HD13	2.49	0.47
1:C:90:GLN:HE21	1:C:93:ASN:H	1.63	0.47
1:C:125:GLN:C	1:C:127:LYS:H	2.16	0.47
1:C:124:GLU:CG	1:C:124:GLU:O	2.62	0.47
1:C:116:VAL:HA	1:C:136:LEU:O	2.15	0.47
1:C:165:THR:HG23	2:D:178:PHE:CE2	2.50	0.47
2:D:52:SER:C	2:D:54:ASP:H	2.19	0.46
1:C:54:ARG:HG2	1:C:58:ILE:HB	1.97	0.46
1:C:164:VAL:HG22	1:C:176:LEU:HB2	1.96	0.46
2:D:199:SER:O	2:D:200:SER:C	2.53	0.46
2:D:79:LEU:HD22	2:D:80:TYR:N	2.32	0.45
1:C:21:LEU:O	1:C:72:THR:HA	2.17	0.45
1:C:34:ALA:O	1:C:88:CYS:HA	2.16	0.45
1:C:124:GLU:O	1:C:127:LYS:CG	2.65	0.45
1:C:202:LEU:HB2	1:C:204:SER:O	2.17	0.45
1:C:8:PRO:O	1:C:103:THR:HG23	2.17	0.45
2:D:151:GLY:HA2	2:D:166:TRP:CZ2	2.52	0.44
1:C:114:PRO:HD3	1:C:140:PHE:HB2	1.99	0.44
1:C:116:VAL:CG1	1:C:208:LYS:HG2	2.47	0.44
1:C:90:GLN:HG2	1:C:92:SER:H	1.83	0.44
1:C:139:ASN:HB3	1:C:173:THR:HG21	1.99	0.43
2:D:158:PHE:HA	2:D:159:PRO:HA	1.66	0.43
1:C:116:VAL:HG12	1:C:208:LYS:HG3	1.99	0.43
2:D:32:TYR:CE2	2:D:101:LYS:HD2	2.54	0.43
1:C:127:LYS:HB3	1:C:127:LYS:HE2	1.64	0.43
2:D:29:PHE:CB	2:D:77:ASN:OD1	2.65	0.43
1:C:137:LEU:HD22	1:C:176:LEU:HG	1.99	0.43
2:D:22:CYS:CB	2:D:79:LEU:HD12	2.49	0.43
2:D:149:ALA:HB2	2:D:195:THR:HG22	2.01	0.43
2:D:60:TYR:CZ	2:D:70:ILE:HG22	2.54	0.43
2:D:156:ASP:HB3	2:D:187:LEU:HD13	2.01	0.42
1:C:80:PRO:HA	1:C:83:PHE:HD2	1.84	0.42
1:C:127:LYS:HG2	1:C:127:LYS:H	1.36	0.42
2:D:22:CYS:HB3	2:D:79:LEU:HB3	2.02	0.42
2:D:207:ILE:HG12	2:D:222:LYS:HA	2.02	0.42
2:D:30:SER:HB2	3:D:273:HOH:O	2.20	0.41
1:C:155:LEU:HD12	1:C:156:GLN:N	2.35	0.41
2:D:160:GLU:HA	2:D:161:PRO:HA	1.63	0.41
1:C:61:ARG:NE	1:C:79:GLU:HG2	2.35	0.41
1:C:200:GLN:NE2	3:C:226:HOH:O	2.35	0.41
1:C:196:GLU:HG3	1:C:207:THR:OG1	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:199:SER:O	2:D:200:SER:O	2.38	0.41
1:C:91:ARG:NH1	2:D:109:SER:HB2	2.36	0.41
1:C:181:THR:HG22	1:C:182:LEU:N	2.36	0.41
2:D:183:GLN:HG3	2:D:183:GLN:H	1.40	0.41
1:C:58:ILE:HA	1:C:59:PRO:HD3	1.90	0.41
1:C:162:GLU:HB3	3:C:243:HOH:O	2.21	0.41
1:C:116:VAL:HG21	1:C:206:VAL:HG21	2.02	0.40
1:C:125:GLN:C	1:C:127:LYS:N	2.74	0.40
1:C:164:VAL:HG22	1:C:176:LEU:CB	2.52	0.40
2:D:124:SER:OG	3:D:255:HOH:O	2.17	0.40
1:C:126:LEU:HA	1:C:126:LEU:HD23	1.85	0.40
1:C:126:LEU:O	1:C:184:LYS:HD3	2.17	0.40
1:C:182:LEU:HD22	1:C:183:SER:N	2.37	0.40

All (5) 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)
2:D:53:TYR:OH	2:D:216:ASN:ND2[4_546]	0.45	1.75
2:D:53:TYR:OH	2:D:216:ASN:CG[4_546]	1.12	1.08
2:D:53:TYR:CZ	2:D:216:ASN:ND2[4_546]	1.27	0.93
2:D:53:TYR:OH	2:D:216:ASN:OD1[4_546]	1.82	0.38
2:D:53:TYR:CE1	2:D:216:ASN:ND2[4_546]	2.00	0.20

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	C	210/216 (97%)	180 (86%)	22 (10%)	8 (4%)	4	3
2	D	202/242 (84%)	180 (89%)	11 (5%)	11 (5%)	2	1
All	All	412/458 (90%)	360 (87%)	33 (8%)	19 (5%)	3	2

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	81	GLU
1	C	123	ASP
2	D	28	THR
2	D	53	TYR
2	D	88	ALA
2	D	183	GLN
2	D	199	SER
2	D	200	SER
1	C	115	SER
1	C	200	GLN
2	D	185	SER
2	D	201	LEU
2	D	203	THR
1	C	126	LEU
1	C	203	SER
1	C	139	ASN
2	D	156	ASP
1	C	44	PRO
2	D	161	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	185/188 (98%)	139 (75%)	46 (25%)	1	1
2	D	174/202 (86%)	137 (79%)	37 (21%)	1	1
All	All	359/390 (92%)	276 (77%)	83 (23%)	1	1

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	4	LEU
1	C	7	SER
1	C	10	THR
1	C	13	LEU

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Mol	Chain	Res	Type
1	C	18	ARG
1	C	22	SER
1	C	31	SER
1	C	33	LEU
1	C	54	ARG
1	C	67	SER
1	C	70	ASP
1	C	74	THR
1	C	75	ILE
1	C	77	SER
1	C	81	GLU
1	C	90	GLN
1	C	93	ASN
1	C	97	ILE
1	C	101	GLN
1	C	104	ARG
1	C	105	LEU
1	C	109	ARG
1	C	110	THR
1	C	127	LYS
1	C	128	SER
1	C	130	THR
1	C	133	VAL
1	C	134	VAL
1	C	138	ASN
1	C	143	ARG
1	C	144	GLU
1	C	148	GLN
1	C	150	LYS
1	C	155	LEU
1	C	157	SER
1	C	159	ASN
1	C	163	SER
1	C	171	ASP
1	C	173	THR
1	C	176	LEU
1	C	182	LEU
1	C	183	SER
1	C	189	LYS
1	C	191	LYS
1	C	200	GLN
1	C	202	LEU

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Mol	Chain	Res	Type
2	D	1	GLN
2	D	12	VAL
2	D	16	ARG
2	D	18	LEU
2	D	20	LEU
2	D	25	SER
2	D	28	THR
2	D	31	SER
2	D	43	LYS
2	D	51	ILE
2	D	53	TYR
2	D	65	LYS
2	D	72	ARG
2	D	75	SER
2	D	76	LYS
2	D	78	THR
2	D	79	LEU
2	D	85	SER
2	D	87	ARG
2	D	109	SER
2	D	124	SER
2	D	127	SER
2	D	129	LYS
2	D	132	SER
2	D	162	VAL
2	D	164	VAL
2	D	165	SER
2	D	172	THR
2	D	182	LEU
2	D	183	GLN
2	D	184	SER
2	D	188	TYR
2	D	190	LEU
2	D	192	SER
2	D	199	SER
2	D	200	SER
2	D	209	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	125	GLN

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Mol	Chain	Res	Type
1	C	138	ASN
1	C	156	GLN
1	C	159	ASN
1	C	167	GLN
1	C	190	HIS
1	C	211	ASN
2	D	204	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 carbohydrates in this entry.

5.6   Ligand geometry (i)

There are no ligands in this entry.

5.7   Other polymers (i)

There are no such residues in this entry.

5.8   Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	C	212/216 (98%)	-0.23	0	100	100	8, 20, 31, 39	0
2	D	208/242 (85%)	-0.05	2 (0%)	84	83	11, 24, 41, 48	0
All	All	420/458 (91%)	-0.14	2 (0%)	91	91	8, 22, 39, 48	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	53	TYR	2.8
2	D	78	THR	2.4

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.