



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:44 PM UTC

PDB ID : 8Q5D / pdb_00008q5d
Title : PfRH5 bound to monoclonal antibody MAD10-466
Authors : Farrell, B.; Higgins, M.K.
Deposited on : 2023-08-08
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

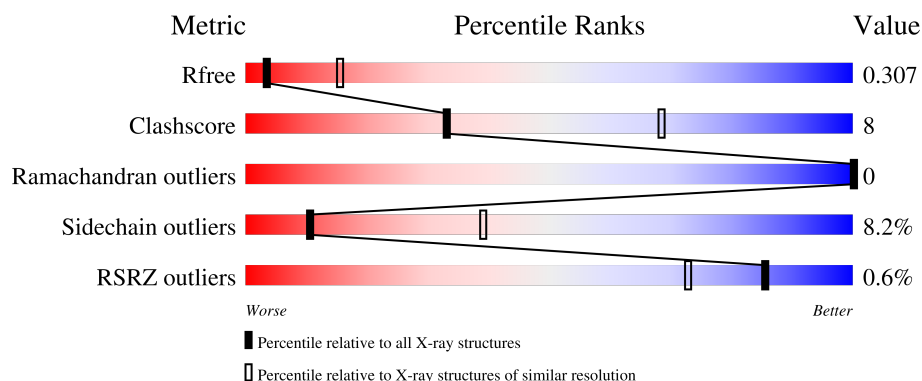
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	338	
1	D	338	
2	B	221	
2	E	221	
3	C	215	

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Mol	Chain	Length	Quality of chain
3	F	215	% 72% 23% . .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11181 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 Reticulocyte-binding protein homolog 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2406	1555	403	435	13			
1	D	278	Total	C	N	O	S	0	0	0
			2363	1525	397	428	13			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	TYR	CYS	engineered mutation	UNP Q8IFM5
A	216	ALA	THR	engineered mutation	UNP Q8IFM5
A	299	ALA	THR	engineered mutation	UNP Q8IFM5
D	203	TYR	CYS	engineered mutation	UNP Q8IFM5
D	216	ALA	THR	engineered mutation	UNP Q8IFM5
D	299	ALA	THR	engineered mutation	UNP Q8IFM5

- Molecule 2 is a protein called Monoclonal antibody MAD10-466 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	0	0
			1571	992	265	307	7			
2	E	213	Total	C	N	O	S	0	0	0
			1586	1001	268	310	7			

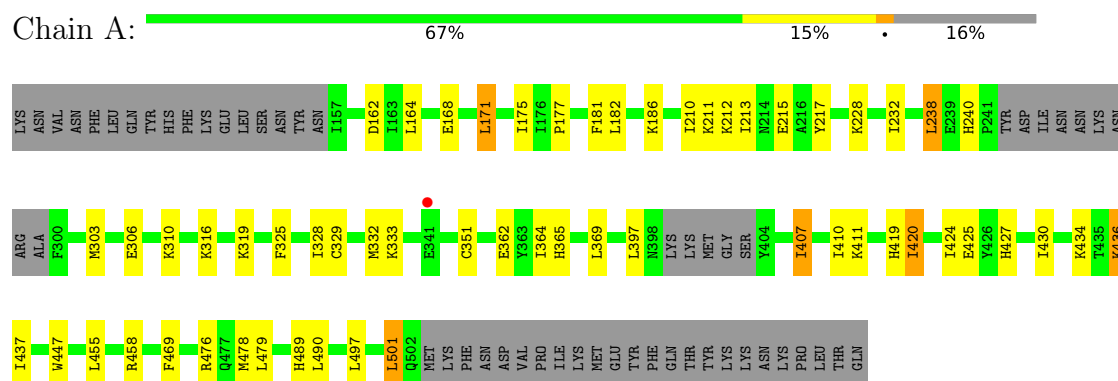
- Molecule 3 is a protein called Monoclonal antibody MAD10-466 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	210	Total	C	N	O	S	0	0	0
			1618	1009	271	333	5			
3	F	212	Total	C	N	O	S	0	0	0
			1637	1019	277	336	5			

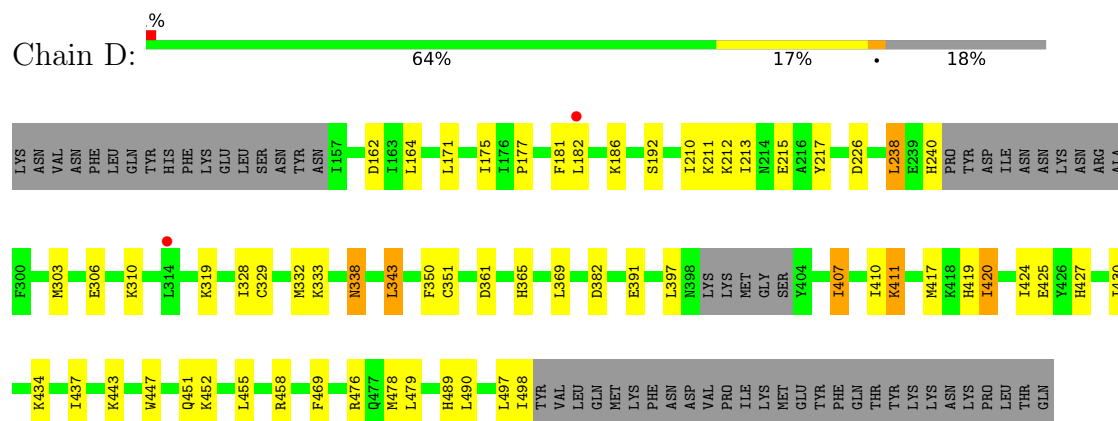
3 Residue-property plots

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.

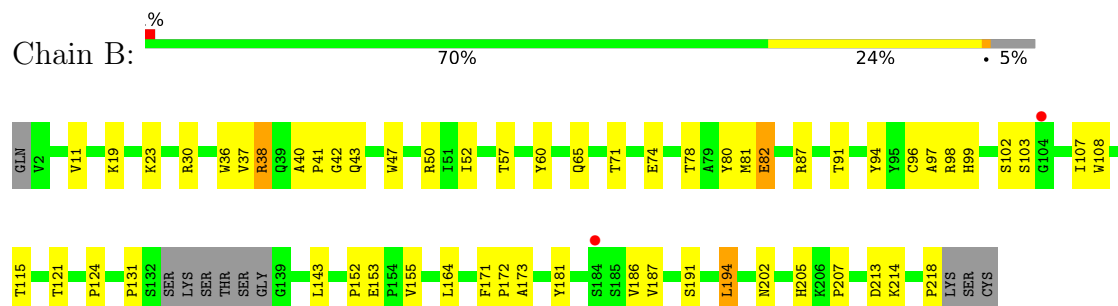
• Molecule 1: Reticulocyte-binding protein homolog 5



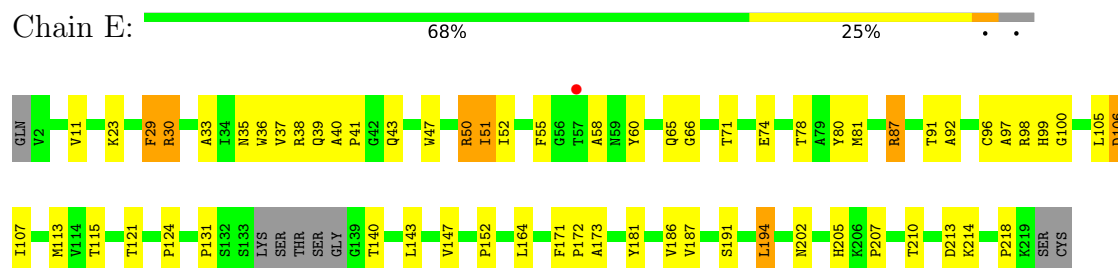
• Molecule 1: Reticulocyte-binding protein homolog 5



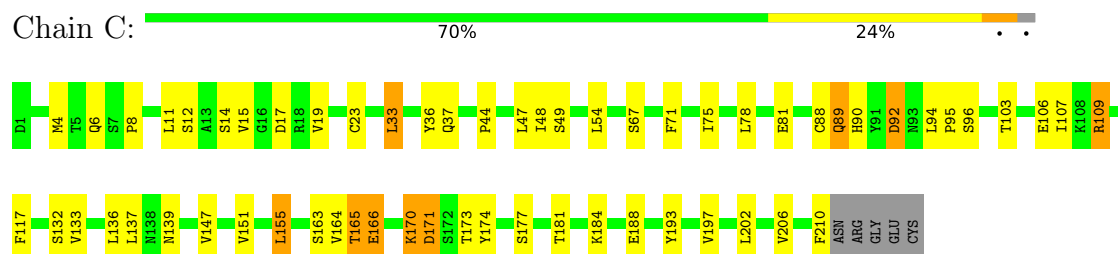
• Molecule 2: Monoclonal antibody MAD10-466 heavy chain



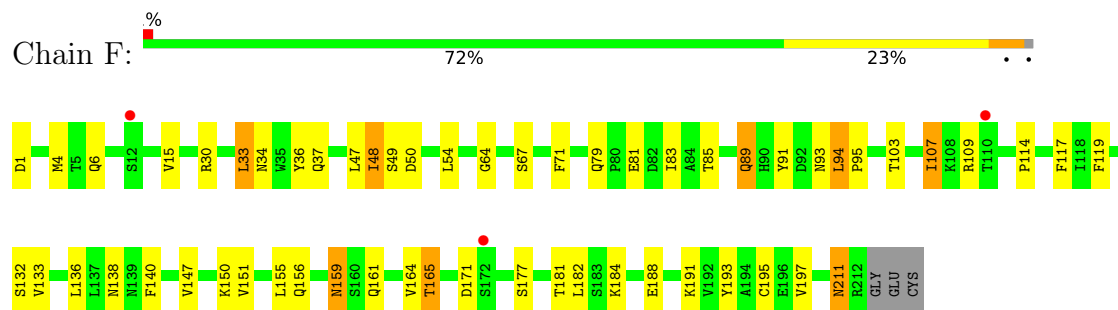
- Molecule 2: Monoclonal antibody MAD10-466 heavy chain



- Molecule 3: Monoclonal antibody MAD10-466 light chain



- Molecule 3: Monoclonal antibody MAD10-466 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.46Å 140.41Å 83.62Å 90.00° 112.74° 90.00°	Depositor
Resolution (Å)	67.59 – 3.20 67.59 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (67.59-3.20) 98.7 (67.59-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 3.19Å)	Xtriage
Refinement program	BUSTER 2.10.4 (26-JUL-2023)	Depositor
R, R_{free}	0.272 , 0.317 0.264 , 0.307	Depositor DCC
R_{free} test set	1464 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	74.0	Xtriage
Anisotropy	0.264	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 85.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.36$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.096 for l,-k,h	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	11181	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.61	0/2456	1.17	5/3296 (0.2%)
1	D	0.61	0/2411	1.18	5/3233 (0.2%)
2	B	0.64	0/1607	1.05	2/2188 (0.1%)
2	E	0.63	0/1622	1.00	1/2207 (0.0%)
3	C	0.66	0/1654	1.08	7/2249 (0.3%)
3	F	0.67	0/1673	1.05	6/2274 (0.3%)
All	All	0.64	0/11423	1.10	26/15447 (0.2%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	419	HIS	CA-C-N	7.41	129.84	122.66
1	D	419	HIS	C-N-CA	7.41	129.84	122.66
1	A	419	HIS	CA-C-N	7.37	129.81	122.66
1	A	419	HIS	C-N-CA	7.37	129.81	122.66
1	D	420	ILE	N-CA-C	-7.07	106.17	111.90
1	A	420	ILE	N-CA-C	-7.03	106.21	111.90
1	D	338	ASN	CA-CB-CG	6.88	119.48	112.60
2	E	29	PHE	CA-CB-CG	6.35	120.15	113.80
3	C	170	LYS	CA-C-N	6.12	131.85	122.23
3	C	170	LYS	C-N-CA	6.12	131.85	122.23
3	F	50	ASP	CA-C-N	5.77	132.56	121.54
3	F	50	ASP	C-N-CA	5.77	132.56	121.54
3	C	75	ILE	CA-C-N	5.37	127.78	120.54
3	C	75	ILE	C-N-CA	5.37	127.78	120.54
3	C	171	ASP	CA-CB-CG	5.30	117.90	112.60
1	A	325	PHE	CA-CB-CG	5.26	119.06	113.80
3	F	188	GLU	CA-C-N	5.25	127.32	120.28
3	F	188	GLU	C-N-CA	5.25	127.32	120.28
1	A	364	ILE	N-CA-C	5.20	116.03	111.56
2	B	42	GLY	CA-C-N	5.20	128.23	120.90
2	B	42	GLY	C-N-CA	5.20	128.23	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	171	ASP	CA-C-N	5.19	130.21	122.74
3	F	171	ASP	C-N-CA	5.19	130.21	122.74
3	C	188	GLU	CA-C-N	5.18	127.22	120.28
3	C	188	GLU	C-N-CA	5.18	127.22	120.28
1	D	382	ASP	CA-CB-CG	5.12	117.72	112.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2406	0	2424	29	0
1	D	2363	0	2380	32	0
2	B	1571	0	1550	36	0
2	E	1586	0	1568	37	0
3	C	1618	0	1555	34	0
3	F	1637	0	1574	26	0
All	All	11181	0	11051	173	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 8.

All (173) 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:B:171:PHE:HB3	3:C:164:VAL:HG11	1.48	0.95
2:E:171:PHE:HB3	3:F:164:VAL:HG11	1.57	0.84
2:E:40:ALA:HB3	2:E:43:GLN:HB2	1.63	0.80
1:D:238:LEU:HG	1:D:303:MET:HG3	1.66	0.77
3:C:37:GLN:HB2	3:C:47:LEU:HD11	1.69	0.75
2:B:40:ALA:HB3	2:B:43:GLN:HB2	1.72	0.72
2:E:43:GLN:H	2:E:43:GLN:CD	1.98	0.72
1:D:417:MET:HE1	1:D:490:LEU:HD22	1.73	0.70
3:C:36:TYR:HE1	3:C:89:GLN:HG2	1.54	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43:GLN:H	2:B:43:GLN:CD	1.99	0.70
3:F:83:ILE:HG12	3:F:107:ILE:HG13	1.75	0.69
3:C:4:MET:HE1	3:C:33:LEU:HD21	1.75	0.69
1:D:238:LEU:HG	1:D:303:MET:CG	2.22	0.69
1:A:238:LEU:HG	1:A:303:MET:HG2	1.75	0.69
2:E:121:THR:HG22	2:E:152:PRO:HD3	1.74	0.69
3:F:150:LYS:HG2	3:F:155:LEU:HG	1.75	0.68
2:B:38:ARG:NH1	2:B:94:TYR:OH	2.28	0.66
2:E:60:TYR:HB2	2:E:65:GLN:HG3	1.78	0.65
2:B:60:TYR:HB2	2:B:65:GLN:HG3	1.78	0.65
3:F:164:VAL:HB	3:F:177:SER:HB3	1.80	0.64
1:A:164:LEU:HG	1:A:478:MET:HB3	1.81	0.63
2:E:173:ALA:HB1	2:E:181:TYR:HB3	1.81	0.63
3:C:164:VAL:HB	3:C:177:SER:HB3	1.80	0.63
2:B:121:THR:HG22	2:B:152:PRO:HD3	1.80	0.62
1:A:365:HIS:NE2	1:A:369:LEU:HD11	2.15	0.61
2:E:172:PRO:HG3	3:F:165:THR:HB	1.82	0.60
1:D:365:HIS:NE2	1:D:369:LEU:HD11	2.16	0.60
3:C:155:LEU:HD13	3:C:155:LEU:H	1.66	0.60
3:C:14:SER:O	3:C:17:ASP:HB2	2.03	0.59
2:B:19:LYS:HG3	2:B:82:GLU:HG3	1.84	0.59
1:A:365:HIS:CD2	2:B:30:ARG:HG2	2.38	0.59
2:E:98:ARG:HE	2:E:100:GLY:HA2	1.68	0.59
3:F:37:GLN:HB2	3:F:47:LEU:HD11	1.84	0.58
2:E:37:VAL:HG22	2:E:47:TRP:HA	1.85	0.58
2:B:99:HIS:CE1	2:B:103:SER:HA	2.39	0.58
3:C:166:GLU:HB2	3:C:174:TYR:HD1	1.69	0.57
2:B:37:VAL:HG22	2:B:47:TRP:HA	1.86	0.57
3:C:147:VAL:HG22	3:C:197:VAL:HG22	1.87	0.56
1:A:210:ILE:HG12	1:A:332:MET:HE1	1.88	0.56
3:F:48:ILE:HG21	3:F:64:GLY:HA3	1.87	0.56
3:F:147:VAL:HG22	3:F:197:VAL:HG22	1.85	0.56
1:A:436:LYS:HZ3	1:D:451:GLN:H	1.54	0.56
3:F:4:MET:HE1	3:F:33:LEU:HD21	1.89	0.55
3:F:34:ASN:HD22	3:F:49:SER:HA	1.69	0.55
3:C:8:PRO:HG3	3:C:11:LEU:HD13	1.87	0.55
1:D:210:ILE:HG12	1:D:332:MET:HE1	1.89	0.55
2:B:172:PRO:HG3	3:C:165:THR:HB	1.89	0.54
3:F:36:TYR:HE1	3:F:89:GLN:HG2	1.72	0.54
1:A:397:LEU:HB3	1:A:407:ILE:HD11	1.89	0.54
3:C:166:GLU:HB2	3:C:174:TYR:CD1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:91:THR:HG23	2:E:115:THR:HA	1.88	0.53
2:B:23:LYS:HG2	2:B:78:THR:HG23	1.91	0.53
1:A:424:ILE:HG12	1:A:479:LEU:HB3	1.91	0.53
2:B:19:LYS:NZ	2:E:66:GLY:H	2.08	0.52
1:D:350:PHE:CD2	3:F:30:ARG:NH1	2.77	0.52
2:B:91:THR:HG23	2:B:115:THR:HA	1.91	0.51
1:A:240:HIS:NE2	1:A:489:HIS:CE1	2.79	0.51
1:D:240:HIS:NE2	1:D:489:HIS:CE1	2.78	0.51
2:E:131:PRO:HD2	2:E:218:PRO:HA	1.92	0.51
2:B:173:ALA:HB1	2:B:181:TYR:HB3	1.93	0.51
3:C:15:VAL:HG23	3:C:107:ILE:HG21	1.93	0.51
1:D:186:LYS:HG3	1:D:210:ILE:HD13	1.92	0.50
1:D:424:ILE:HG12	1:D:479:LEU:HB3	1.92	0.50
2:E:202:ASN:ND2	2:E:213:ASP:OD1	2.45	0.50
2:E:35:ASN:HB2	2:E:97:ALA:HB3	1.93	0.50
3:F:94:LEU:N	3:F:95:PRO:HA	2.26	0.50
2:E:23:LYS:HG2	2:E:78:THR:HG23	1.93	0.50
2:B:131:PRO:HD2	2:B:218:PRO:HA	1.93	0.49
1:A:181:PHE:HZ	1:A:333:LYS:HB2	1.77	0.49
2:E:43:GLN:CD	2:E:43:GLN:N	2.69	0.49
1:A:182:LEU:HD21	1:A:329:CYS:HA	1.94	0.49
2:B:43:GLN:CD	2:B:43:GLN:N	2.69	0.49
2:B:202:ASN:ND2	2:B:213:ASP:OD1	2.45	0.49
1:D:447:TRP:HZ3	2:E:99:HIS:CD2	2.29	0.49
3:F:114:PRO:HA	3:F:140:PHE:HB3	1.94	0.49
2:B:57:THR:HG22	2:E:55:PHE:HA	1.95	0.49
1:D:410:ILE:HG23	1:D:490:LEU:HD11	1.94	0.49
2:B:97:ALA:HA	2:B:107:ILE:O	2.13	0.49
1:D:181:PHE:HZ	1:D:333:LYS:HB2	1.77	0.49
2:B:71:THR:HG23	2:B:80:TYR:HD2	1.78	0.49
2:E:164:LEU:HD21	2:E:187:VAL:HG21	1.95	0.49
3:C:15:VAL:HG22	3:C:107:ILE:HD13	1.95	0.48
2:E:186:VAL:HG21	3:F:136:LEU:HD22	1.95	0.48
1:D:417:MET:CE	1:D:490:LEU:HD22	2.42	0.48
1:A:410:ILE:HG23	1:A:490:LEU:HD11	1.95	0.48
3:F:191:LYS:O	3:F:211:ASN:HA	2.14	0.48
1:A:186:LYS:HG3	1:A:210:ILE:HD13	1.95	0.48
1:A:365:HIS:CD2	1:A:369:LEU:HD11	2.48	0.48
2:B:71:THR:HG22	2:B:82:GLU:OE1	2.14	0.48
1:D:182:LEU:HD21	1:D:329:CYS:HA	1.95	0.47
1:D:192:SER:HA	1:D:343:LEU:HD21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:71:THR:HG23	2:E:80:TYR:HD2	1.78	0.47
1:A:181:PHE:CZ	1:A:333:LYS:HB2	2.49	0.47
1:A:351:CYS:HB3	1:A:455:LEU:HD22	1.96	0.47
3:C:137:LEU:HD11	3:C:147:VAL:HG21	1.96	0.47
1:A:447:TRP:HZ3	2:B:99:HIS:ND1	2.13	0.47
1:D:365:HIS:CD2	1:D:369:LEU:HD11	2.49	0.47
1:A:306:GLU:HG2	1:A:310:LYS:HE2	1.97	0.46
1:D:306:GLU:HG2	1:D:310:LYS:HE2	1.98	0.46
1:D:181:PHE:CZ	1:D:333:LYS:HB2	2.50	0.46
1:D:351:CYS:HB3	1:D:455:LEU:HD22	1.97	0.46
2:E:131:PRO:HA	3:F:119:PHE:HE1	1.80	0.46
1:D:361:ASP:OD1	2:E:30:ARG:HB2	2.16	0.46
2:B:11:VAL:HB	2:B:152:PRO:HG3	1.97	0.46
3:F:6:GLN:NE2	3:F:103:THR:OG1	2.48	0.46
2:B:102:SER:HB2	3:C:49:SER:HB2	1.97	0.46
3:C:94:LEU:N	3:C:95:PRO:HA	2.30	0.46
2:B:164:LEU:HD21	2:B:187:VAL:HG21	1.97	0.45
3:C:12:SER:HA	3:C:106:GLU:O	2.16	0.45
1:D:240:HIS:NE2	1:D:489:HIS:NE2	2.64	0.45
2:E:172:PRO:CG	3:F:165:THR:HB	2.45	0.45
1:D:175:ILE:HG22	1:D:177:PRO:HD2	1.99	0.45
2:E:30:ARG:H	2:E:30:ARG:HG2	1.46	0.45
1:A:436:LYS:HE2	1:D:451:GLN:HB2	1.97	0.45
2:E:39:GLN:O	2:E:92:ALA:HB1	2.17	0.45
3:C:132:SER:HA	3:C:181:THR:HA	1.99	0.45
3:F:132:SER:HA	3:F:181:THR:HA	1.99	0.45
1:A:240:HIS:NE2	1:A:489:HIS:NE2	2.65	0.45
2:E:205:HIS:CD2	2:E:207:PRO:HD2	2.52	0.44
3:C:139:ASN:HA	3:C:173:THR:HB	1.98	0.44
3:F:79:GLN:OE1	3:F:81:GLU:OE1	2.35	0.44
1:A:175:ILE:HG22	1:A:177:PRO:HD2	2.00	0.44
2:B:205:HIS:CD2	2:B:207:PRO:HD2	2.53	0.44
3:C:92:ASP:HB3	3:C:94:LEU:HG	1.99	0.44
3:C:81:GLU:HA	3:C:170:LYS:HG2	2.00	0.44
3:C:109:ARG:HA	3:C:109:ARG:HD2	1.71	0.44
2:B:40:ALA:HB1	2:B:41:PRO:CD	2.49	0.43
3:C:67:SER:HA	3:C:71:PHE:CE2	2.53	0.43
1:D:217:TYR:HA	1:D:328:ILE:HD13	2.00	0.43
2:E:36:TRP:CE2	2:E:81:MET:HB2	2.54	0.43
2:B:191:SER:HA	2:B:194:LEU:HD22	2.00	0.43
2:B:124:PRO:HG3	2:B:205:HIS:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:GLN:NE2	3:C:103:THR:OG1	2.50	0.43
2:E:33:ALA:HB1	2:E:50:ARG:HD2	1.99	0.43
3:F:67:SER:HA	3:F:71:PHE:CE2	2.54	0.43
3:C:171:ASP:O	3:C:171:ASP:OD1	2.36	0.42
2:E:100:GLY:CA	2:E:106:ASP:HB2	2.49	0.42
3:C:202:LEU:HD13	3:C:206:VAL:HG22	2.01	0.42
3:C:33:LEU:HD11	3:C:88:CYS:HB2	2.01	0.42
1:D:397:LEU:HB3	1:D:407:ILE:HD11	2.01	0.42
1:D:407:ILE:HG23	1:D:411:LYS:HE3	2.02	0.42
2:E:191:SER:HA	2:E:194:LEU:HD22	2.00	0.42
2:B:102:SER:HB2	3:C:49:SER:CB	2.50	0.42
1:A:217:TYR:HA	1:A:328:ILE:HD13	2.01	0.42
2:B:36:TRP:CE2	2:B:81:MET:HB2	2.54	0.42
1:D:164:LEU:HG	1:D:478:MET:HB3	2.02	0.42
1:D:212:LYS:HA	1:D:215:GLU:HB2	2.01	0.42
1:A:447:TRP:HZ3	2:B:99:HIS:HD1	1.67	0.42
1:D:427:HIS:HA	1:D:430:ILE:HD12	2.02	0.42
2:B:19:LYS:HG3	2:B:82:GLU:CG	2.48	0.42
2:B:186:VAL:HG21	3:C:136:LEU:HD22	2.01	0.42
3:F:156:GLN:HB3	3:F:159:ASN:ND2	2.35	0.42
1:A:212:LYS:HA	1:A:215:GLU:HB2	2.02	0.41
3:F:91:TYR:CZ	3:F:93:ASN:HA	2.56	0.41
2:E:124:PRO:HD2	2:E:210:THR:HG21	2.03	0.41
2:B:108:TRP:CE3	3:C:44:PRO:HD2	2.55	0.41
3:F:151:VAL:HG13	3:F:193:TYR:CE1	2.56	0.41
1:A:228:LYS:O	1:A:232:ILE:HG13	2.20	0.41
1:A:497:LEU:HD12	1:A:501:LEU:HD22	2.02	0.41
1:A:171:LEU:HB2	1:A:232:ILE:HG12	2.02	0.41
3:C:4:MET:HE3	3:C:23:CYS:SG	2.61	0.41
3:C:193:TYR:HB2	3:C:210:PHE:CE1	2.55	0.41
2:E:40:ALA:HB1	2:E:41:PRO:CD	2.51	0.41
1:A:427:HIS:HA	1:A:430:ILE:HD12	2.02	0.40
3:C:151:VAL:HG13	3:C:193:TYR:CE1	2.56	0.40
1:D:424:ILE:CG1	1:D:479:LEU:HB3	2.51	0.40
2:E:87:ARG:HH11	2:E:87:ARG:HB2	1.85	0.40
2:E:124:PRO:HB2	2:E:147:VAL:HG13	2.01	0.40
1:D:434:LYS:HB3	1:D:469:PHE:HB2	2.02	0.40
3:F:147:VAL:HG13	3:F:195:CYS:HB2	2.03	0.40
2:E:51:ILE:HD12	2:E:58:ALA:HB2	2.02	0.40
1:A:434:LYS:HB3	1:A:469:PHE:HB2	2.02	0.40
2:E:11:VAL:HB	2:E:152:PRO:HG3	2.03	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	277/338 (82%)	269 (97%)	8 (3%)	0	100	100
1	D	272/338 (80%)	265 (97%)	7 (3%)	0	100	100
2	B	207/221 (94%)	184 (89%)	23 (11%)	0	100	100
2	E	209/221 (95%)	187 (90%)	22 (10%)	0	100	100
3	C	208/215 (97%)	183 (88%)	25 (12%)	0	100	100
3	F	210/215 (98%)	186 (89%)	24 (11%)	0	100	100
All	All	1383/1548 (89%)	1274 (92%)	109 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	274/327 (84%)	256 (93%)	18 (7%)	15	47
1	D	269/327 (82%)	248 (92%)	21 (8%)	11	41
2	B	176/185 (95%)	163 (93%)	13 (7%)	13	43
2	E	178/185 (96%)	161 (90%)	17 (10%)	8	32
3	C	187/191 (98%)	170 (91%)	17 (9%)	9	34
3	F	189/191 (99%)	170 (90%)	19 (10%)	7	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1273/1406 (90%)	1168 (92%)	105 (8%)	10	39

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	ASP
1	A	168	GLU
1	A	171	LEU
1	A	211	LYS
1	A	213	ILE
1	A	238	LEU
1	A	316	LYS
1	A	319	LYS
1	A	362	GLU
1	A	407	ILE
1	A	411	LYS
1	A	420	ILE
1	A	425	GLU
1	A	436	LYS
1	A	437	ILE
1	A	458	ARG
1	A	476	ARG
1	A	501	LEU
2	B	38	ARG
2	B	50	ARG
2	B	52	ILE
2	B	74	GLU
2	B	82	GLU
2	B	87	ARG
2	B	96	CYS
2	B	98	ARG
2	B	143	LEU
2	B	153	GLU
2	B	155	VAL
2	B	194	LEU
2	B	214	LYS
3	C	19	VAL
3	C	33	LEU
3	C	48	ILE
3	C	54	LEU
3	C	78	LEU
3	C	89	GLN

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Mol	Chain	Res	Type
3	C	90	HIS
3	C	92	ASP
3	C	96	SER
3	C	109	ARG
3	C	117	PHE
3	C	133	VAL
3	C	155	LEU
3	C	163	SER
3	C	165	THR
3	C	166	GLU
3	C	184	LYS
1	D	162	ASP
1	D	171	LEU
1	D	211	LYS
1	D	213	ILE
1	D	226	ASP
1	D	238	LEU
1	D	319	LYS
1	D	338	ASN
1	D	343	LEU
1	D	391	GLU
1	D	407	ILE
1	D	411	LYS
1	D	420	ILE
1	D	425	GLU
1	D	437	ILE
1	D	443	LYS
1	D	452	LYS
1	D	458	ARG
1	D	476	ARG
1	D	497	LEU
1	D	498	ILE
2	E	29	PHE
2	E	30	ARG
2	E	38	ARG
2	E	50	ARG
2	E	51	ILE
2	E	52	ILE
2	E	74	GLU
2	E	87	ARG
2	E	96	CYS
2	E	105	LEU

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Mol	Chain	Res	Type
2	E	106	ASP
2	E	107	ILE
2	E	113	MET
2	E	140	THR
2	E	143	LEU
2	E	194	LEU
2	E	214	LYS
3	F	1	ASP
3	F	15	VAL
3	F	33	LEU
3	F	48	ILE
3	F	54	LEU
3	F	85	THR
3	F	89	GLN
3	F	94	LEU
3	F	107	ILE
3	F	109	ARG
3	F	117	PHE
3	F	133	VAL
3	F	138	ASN
3	F	159	ASN
3	F	161	GLN
3	F	165	THR
3	F	182	LEU
3	F	184	LYS
3	F	211	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	225	ASN
1	A	308	ASN
1	A	354	ASN
1	A	398	ASN
1	A	427	HIS
2	B	99	HIS
2	B	169	HIS
2	B	176	GLN
3	C	6	GLN
3	C	34	ASN
3	C	89	GLN
3	C	138	ASN

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Mol	Chain	Res	Type
3	C	200	GLN
1	D	225	ASN
1	D	308	ASN
1	D	354	ASN
1	D	398	ASN
1	D	427	HIS
2	E	59	ASN
3	F	34	ASN
3	F	89	GLN
3	F	138	ASN
3	F	139	ASN
3	F	153	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	283/338 (83%)	-0.09	1 (0%) 88 79	65, 93, 122, 156	0
1	D	278/338 (82%)	-0.04	2 (0%) 84 69	58, 92, 139, 150	0
2	B	211/221 (95%)	-0.04	2 (0%) 81 64	66, 86, 122, 131	0
2	E	213/221 (96%)	0.06	1 (0%) 87 76	64, 90, 157, 170	0
3	C	210/215 (97%)	0.20	0 100 100	75, 107, 141, 148	0
3	F	212/215 (98%)	0.20	3 (1%) 73 54	62, 104, 149, 156	0
All	All	1407/1548 (90%)	0.04	9 (0%) 85 73	58, 94, 147, 170	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	314	LEU	2.8
2	E	57	THR	2.8
3	F	12	SER	2.5
1	D	182	LEU	2.4
1	A	341	GLU	2.3
3	F	110	THR	2.1
2	B	104	GLY	2.1
2	B	184	SER	2.1
3	F	172	SER	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.