



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:56 AM UTC

PDB ID : 7PHU / pdb_00007phu
Title : PfRH5 bound to monoclonal antibody R5.015 and R5.016 Fab fragments
Authors : Ragotte, R.J.; Higgins, M.K.
Deposited on : 2021-08-18
Resolution : 2.53 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

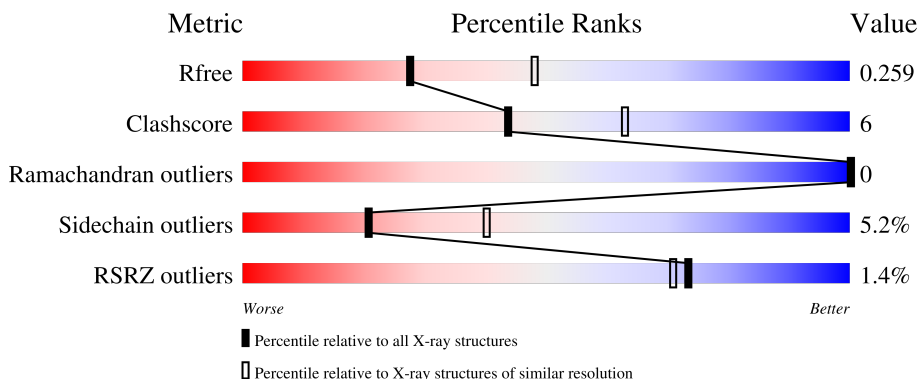
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (2.54-2.50)

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	501	% 48% 10% 41%
2	B	236	2% 78% 16% 6%
3	C	217	88% 8% ..
4	D	464	% 42% 6% 50%
5	E	219	% 77% 18% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9294 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	295	Total	C	N	O	S	0	0	0
			2511	1620	422	453	16			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	38	GLN	ASN	conflict	UNP Q8IFM5
A	203	TYR	CYS	conflict	UNP Q8IFM5
A	216	ALA	THR	conflict	UNP Q8IFM5

- Molecule 2 is a protein called Monoclonal antibody R5.015 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	222	Total	C	N	O	S	0	0	0
			1683	1069	278	327	9			

- Molecule 3 is a protein called Monoclonal antibody R5.015 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	212	Total	C	N	O	S	0	0	0
			1599	1004	266	324	5			

- Molecule 4 is a protein called Monoclonal antibody R5.016 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	232	Total	C	N	O	S	0	0	0
			1746	1098	290	349	9			

- Molecule 5 is a protein called Monoclonal antibody R5.016 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	211	Total 1628	C 1019	N 276	O 328	S 5	0	0	0

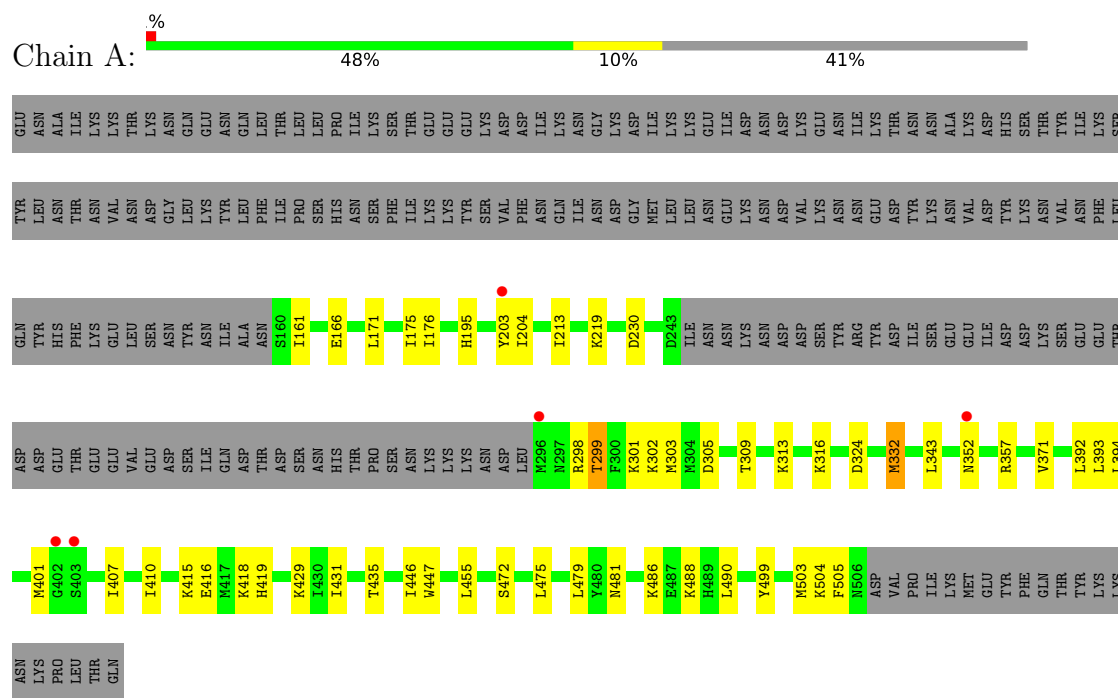
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	31	Total 31	O 31	0	0
6	B	8	Total 8	O 8	0	0
6	C	36	Total 36	O 36	0	0
6	D	27	Total 27	O 27	0	0
6	E	25	Total 25	O 25	0	0

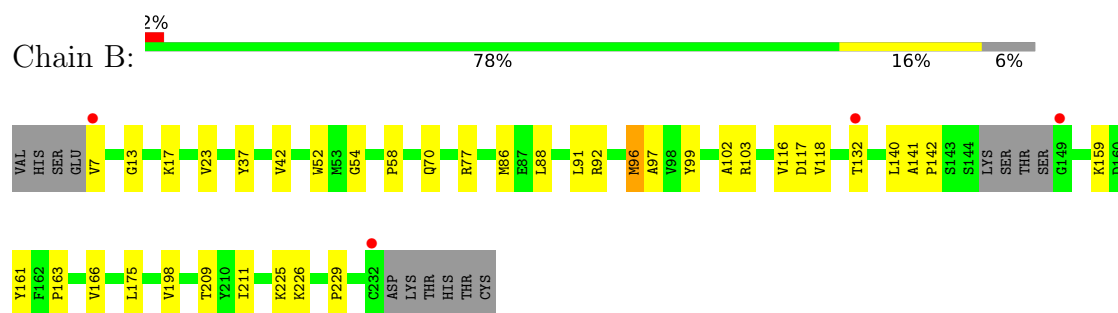
3 Residue-property plots

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 2: Monoclonal antibody R5.015 heavy chain

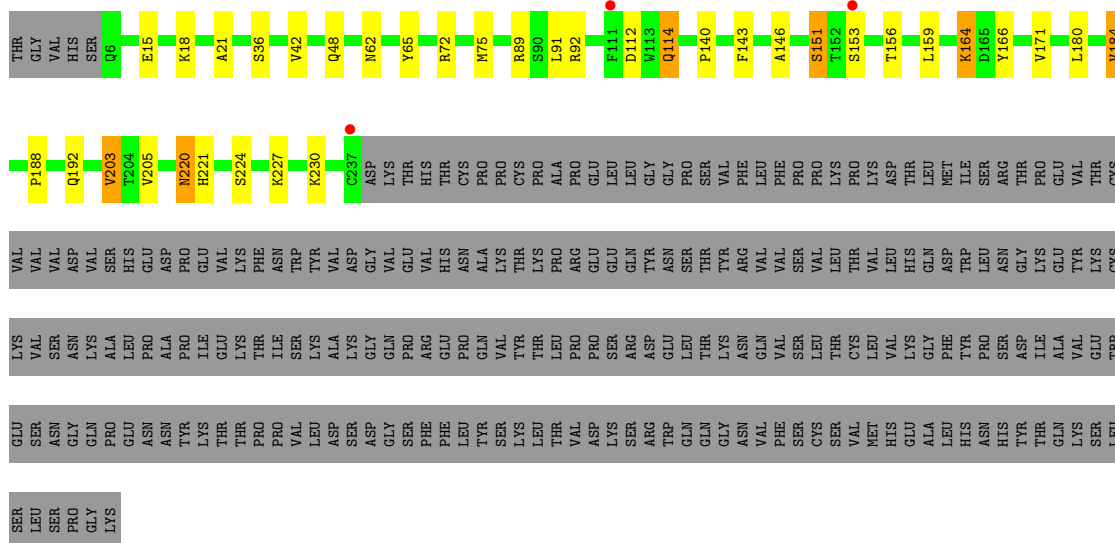
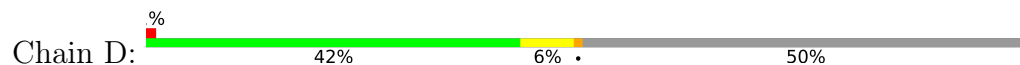


• Molecule 3: Monoclonal antibody R5.015 light chain

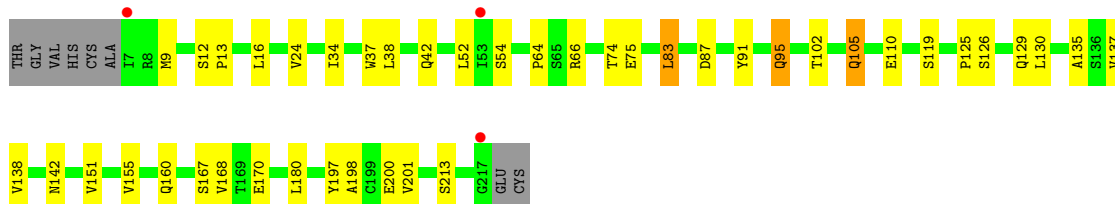
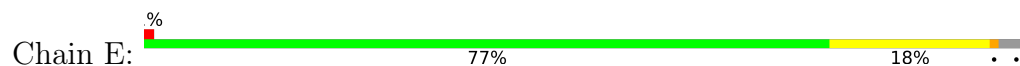




• Molecule 4: Monoclonal antibody R5.016 heavy chain



• Molecule 5: Monoclonal antibody R5.016 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	97.74Å 163.30Å 176.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.79 – 2.53 47.79 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.5 (47.79-2.53) 99.5 (47.79-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 2.54Å)	Xtriage
Refinement program	BUSTER 2.10.4 (24-FEB-2021)	Depositor
R, R_{free}	0.236 , 0.276 0.223 , 0.259	Depositor DCC
R_{free} test set	2354 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	59.9	Xtriage
Anisotropy	0.622	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.001 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9294	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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 [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	A	0.78	1/2564 (0.0%)	1.22	4/3437 (0.1%)
2	B	0.77	0/1730	1.08	5/2362 (0.2%)
3	C	0.76	0/1641	1.09	2/2246 (0.1%)
4	D	0.70	0/1790	1.06	4/2442 (0.2%)
5	E	0.73	0/1663	1.01	0/2258
All	All	0.75	1/9388 (0.0%)	1.11	15/12745 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	332	MET	SD-CE	-8.21	1.59	1.79

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	50	ASP	CA-CB-CG	6.96	119.56	112.60
1	A	324	ASP	CA-CB-CG	6.96	119.56	112.60
4	D	146	ALA	N-CA-C	5.97	117.17	109.65
4	D	151	SER	CA-C-N	5.90	130.80	121.72
4	D	151	SER	C-N-CA	5.90	130.80	121.72
4	D	184	VAL	N-CA-CB	5.71	118.45	110.56
1	A	393	LEU	CA-C-N	5.58	128.07	120.54
1	A	393	LEU	C-N-CA	5.58	128.07	120.54
2	B	117	ASP	CA-CB-CG	5.32	117.92	112.60
2	B	141	ALA	N-CA-C	5.18	115.56	109.60
2	B	209	THR	CB-CA-C	5.09	118.03	109.48
3	C	200	GLU	N-CA-C	-5.08	99.99	110.80
2	B	13	GLY	CA-C-N	5.01	127.97	120.90
2	B	13	GLY	C-N-CA	5.01	127.97	120.90
1	A	299	THR	CA-C-O	-5.01	115.83	122.44

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2511	0	2531	32	0
2	B	1683	0	1624	25	0
3	C	1599	0	1535	10	0
4	D	1746	0	1682	23	0
5	E	1628	0	1584	26	0
6	A	31	0	0	0	0
6	B	8	0	0	0	0
6	C	36	0	0	0	0
6	D	27	0	0	0	0
6	E	25	0	0	0	0
All	All	9294	0	8956	111	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 6.

All (111) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:184:VAL:HG22	4:D:203:VAL:CG1	1.82	1.09
4:D:184:VAL:HG22	4:D:203:VAL:HG12	1.08	1.06
2:B:161:TYR:CE2	2:B:166:VAL:HG23	2.01	0.96
4:D:184:VAL:CG2	4:D:203:VAL:HG12	1.94	0.96
1:A:195:HIS:CD2	1:A:343:LEU:HD11	2.07	0.88
1:A:415:LYS:HA	1:A:418:LYS:HE2	1.59	0.82
3:C:112:LYS:HG2	3:C:143:PRO:HD3	1.62	0.81
1:A:195:HIS:CG	1:A:343:LEU:HD11	2.15	0.81
4:D:21:ALA:O	4:D:91:LEU:HG	1.83	0.79
5:E:155:VAL:HG12	5:E:197:TYR:CD2	2.19	0.78
1:A:299:THR:HG22	1:A:299:THR:O	1.84	0.77
2:B:161:TYR:CE2	2:B:166:VAL:CG2	2.67	0.77
3:C:121:PRO:HB3	3:C:208:VAL:CG1	2.17	0.74
4:D:65:TYR:HE1	4:D:75:MET:HG2	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ARG:HH21	1:A:299:THR:H	1.37	0.71
3:C:121:PRO:HB3	3:C:208:VAL:HG11	1.70	0.71
1:A:176:ILE:HG12	1:A:475:LEU:HD11	1.72	0.70
2:B:86:MET:HE3	2:B:88:LEU:HD11	1.76	0.68
2:B:23:VAL:CG2	2:B:88:LEU:HD13	2.25	0.66
3:C:12:VAL:HG21	3:C:18:ALA:HB2	1.79	0.63
4:D:159:LEU:C	4:D:159:LEU:HD12	2.24	0.62
2:B:102:ALA:HB1	2:B:116:VAL:HG11	1.82	0.61
1:A:298:ARG:HH21	1:A:299:THR:N	1.98	0.61
2:B:23:VAL:HG13	2:B:91:LEU:HD11	1.83	0.61
5:E:42:GLN:HB2	5:E:52:LEU:HD11	1.83	0.60
1:A:166:GLU:HA	1:A:481:ASN:HB3	1.84	0.59
2:B:23:VAL:HG23	2:B:88:LEU:HD13	1.83	0.59
2:B:102:ALA:HB1	2:B:116:VAL:CG1	2.34	0.58
2:B:161:TYR:CD2	2:B:166:VAL:CG2	2.86	0.58
4:D:171:VAL:HG12	4:D:221:HIS:CD2	2.38	0.58
1:A:431:ILE:O	1:A:435:THR:HG23	2.04	0.57
5:E:83:LEU:HD13	5:E:87:ASP:HB2	1.87	0.57
1:A:298:ARG:NH2	1:A:299:THR:HA	2.19	0.56
2:B:7:VAL:CG1	2:B:118:VAL:HG21	2.36	0.55
1:A:499:TYR:CE1	1:A:503:MET:HG3	2.41	0.55
1:A:213:ILE:HG13	1:A:332:MET:HE2	1.88	0.55
5:E:155:VAL:CG1	5:E:197:TYR:CD2	2.91	0.54
2:B:52:TRP:CZ2	2:B:54:GLY:HA2	2.43	0.54
5:E:155:VAL:HG22	5:E:160:GLN:NE2	2.23	0.54
5:E:9:MET:HG2	5:E:102:THR:HG22	1.89	0.53
1:A:195:HIS:CE1	1:A:352:ASN:OD1	2.62	0.53
1:A:371:VAL:HG11	1:A:431:ILE:CG2	2.38	0.53
2:B:17:LYS:HG3	2:B:23:VAL:CG1	2.38	0.53
4:D:184:VAL:CG2	4:D:203:VAL:CG1	2.70	0.53
2:B:86:MET:HE3	2:B:88:LEU:CD1	2.39	0.53
2:B:132:THR:HG22	2:B:163:PRO:HD3	1.91	0.53
5:E:13:PRO:HG3	5:E:16:LEU:HD13	1.91	0.52
5:E:198:ALA:HB2	5:E:213:SER:HB3	1.92	0.51
1:A:415:LYS:O	1:A:419:HIS:CD2	2.63	0.51
2:B:7:VAL:HG11	2:B:118:VAL:HG21	1.92	0.51
5:E:38:LEU:O	5:E:54:SER:O	2.29	0.50
1:A:195:HIS:CD2	1:A:343:LEU:CD1	2.87	0.50
1:A:299:THR:O	1:A:299:THR:CG2	2.53	0.50
5:E:95:GLN:HE21	5:E:102:THR:HB	1.78	0.49
5:E:125:PRO:HD3	5:E:137:VAL:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:119:LEU:HD23	3:C:208:VAL:HG23	1.95	0.49
1:A:305:ASP:O	1:A:309:THR:HG23	2.13	0.48
5:E:34:ILE:HG21	5:E:95:GLN:HG3	1.94	0.48
4:D:143:PHE:CE2	5:E:129:GLN:HG3	2.49	0.48
5:E:66:ARG:HD2	5:E:87:ASP:OD2	2.14	0.48
4:D:140:PRO:HB3	4:D:166:TYR:HB3	1.96	0.47
5:E:151:VAL:HG22	5:E:201:VAL:HG22	1.97	0.47
5:E:168:VAL:HG22	5:E:180:LEU:HD12	1.97	0.47
4:D:114:GLN:HG3	5:E:37:TRP:CE2	2.50	0.46
2:B:37:TYR:O	2:B:58:PRO:HG3	2.14	0.46
4:D:221:HIS:ND1	4:D:224:SER:OG	2.44	0.46
5:E:105:GLN:H	5:E:105:GLN:HG3	1.47	0.45
1:A:299:THR:HG22	1:A:302:LYS:H	1.80	0.45
3:C:14:PRO:O	3:C:77:VAL:O	2.35	0.45
4:D:153:SER:O	4:D:156:THR:HG22	2.15	0.45
4:D:203:VAL:HG23	4:D:205:VAL:HG13	1.98	0.45
1:A:161:ILE:HG12	1:A:175:ILE:HG12	1.98	0.45
5:E:64:PRO:HB2	5:E:66:ARG:HG2	1.97	0.45
1:A:313:LYS:HA	1:A:316:LYS:HE2	1.99	0.45
1:A:352:ASN:OD1	1:A:352:ASN:O	2.34	0.45
1:A:195:HIS:CB	1:A:343:LEU:HD11	2.47	0.45
2:B:211:ILE:HG12	2:B:226:LYS:HG2	1.99	0.45
2:B:175:LEU:HD21	2:B:198:VAL:HG21	1.99	0.45
5:E:126:SER:O	5:E:130:LEU:HG	2.16	0.45
2:B:23:VAL:HG22	2:B:88:LEU:HB2	1.99	0.44
4:D:164:LYS:HE2	4:D:192:GLN:OE1	2.17	0.44
2:B:142:PRO:HD2	2:B:229:PRO:HA	2.00	0.44
1:A:410:ILE:HG23	1:A:490:LEU:HD11	1.99	0.44
1:A:504:LYS:HG2	1:A:505:PHE:H	1.82	0.44
4:D:72:ARG:HG2	4:D:89:ARG:O	2.19	0.43
4:D:220:ASN:OD1	4:D:227:LYS:HG2	2.18	0.43
5:E:119:SER:HB2	5:E:142:ASN:HB3	2.00	0.43
5:E:155:VAL:CG1	5:E:197:TYR:CE2	3.01	0.43
1:A:204:ILE:HD11	4:D:36:SER:HA	2.00	0.43
3:C:119:LEU:HG	3:C:208:VAL:HG21	2.01	0.43
2:B:97:ALA:HB3	2:B:99:TYR:CE1	2.54	0.43
1:A:357:ARG:HG3	1:A:446:ILE:HD11	2.01	0.43
2:B:161:TYR:CE2	2:B:166:VAL:HG21	2.53	0.43
2:B:161:TYR:CD2	2:B:166:VAL:HG21	2.53	0.42
4:D:75:MET:HB3	4:D:75:MET:HE2	1.81	0.42
1:A:475:LEU:O	1:A:479:LEU:HD12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:155:VAL:HG11	5:E:197:TYR:CE2	2.54	0.42
1:A:298:ARG:HH21	1:A:299:THR:CA	2.33	0.42
4:D:65:TYR:CE1	4:D:75:MET:HG2	2.44	0.42
3:C:112:LYS:NZ	3:C:200:GLU:OE1	2.49	0.41
5:E:42:GLN:HG3	5:E:91:TYR:CE2	2.56	0.41
4:D:171:VAL:HG12	4:D:221:HIS:HD2	1.83	0.41
4:D:184:VAL:HG22	4:D:203:VAL:CB	2.46	0.41
5:E:125:PRO:HG3	5:E:135:ALA:HB1	2.02	0.41
1:A:298:ARG:NH2	1:A:299:THR:CA	2.83	0.41
1:A:446:ILE:HG23	1:A:447:TRP:CD1	2.55	0.41
2:B:96:MET:HE3	2:B:96:MET:HB3	1.84	0.41
2:B:140:LEU:HB3	3:C:120:PHE:CD1	2.56	0.40
3:C:22:CYS:HB3	3:C:70:ALA:HB3	2.03	0.40
1:A:416:GLU:OE1	1:A:486:LYS:HE3	2.21	0.40
4:D:188:PRO:O	5:E:167:SER:OG	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	291/501 (58%)	284 (98%)	7 (2%)	0	100	100
2	B	218/236 (92%)	211 (97%)	7 (3%)	0	100	100
3	C	210/217 (97%)	201 (96%)	9 (4%)	0	100	100
4	D	230/464 (50%)	218 (95%)	12 (5%)	0	100	100
5	E	209/219 (95%)	199 (95%)	10 (5%)	0	100	100
All	All	1158/1637 (71%)	1113 (96%)	45 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	286/486 (59%)	272 (95%)	14 (5%)	22	43
2	B	188/202 (93%)	180 (96%)	8 (4%)	26	49
3	C	180/185 (97%)	173 (96%)	7 (4%)	28	52
4	D	195/409 (48%)	181 (93%)	14 (7%)	13	26
5	E	186/192 (97%)	175 (94%)	11 (6%)	18	35
All	All	1035/1474 (70%)	981 (95%)	54 (5%)	21	40

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	171	LEU
1	A	203	TYR
1	A	219	LYS
1	A	230	ASP
1	A	301	LYS
1	A	303	MET
1	A	392	LEU
1	A	394	LEU
1	A	401	MET
1	A	407	ILE
1	A	429	LYS
1	A	455	LEU
1	A	472	SER
1	A	488	LYS
2	B	42	VAL
2	B	70	GLN
2	B	77	ARG
2	B	92	ARG
2	B	96	MET
2	B	103	ARG
2	B	159	LYS
2	B	225	LYS
3	C	25	ASN

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Mol	Chain	Res	Type
3	C	41	GLN
3	C	48	TYR
3	C	59	GLU
3	C	79	VAL
3	C	143	PRO
3	C	182	LEU
4	D	15	GLU
4	D	18	LYS
4	D	42	VAL
4	D	48	GLN
4	D	62	ASN
4	D	92	ARG
4	D	112	ASP
4	D	114	GLN
4	D	151	SER
4	D	164	LYS
4	D	180	LEU
4	D	203	VAL
4	D	220	ASN
4	D	230	LYS
5	E	12	SER
5	E	24	VAL
5	E	74	THR
5	E	75	GLU
5	E	83	LEU
5	E	95	GLN
5	E	105	GLN
5	E	110	GLU
5	E	138	VAL
5	E	170	GLU
5	E	200	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	195	HIS
1	A	297	ASN
1	A	342	GLN
1	A	348	ASN
1	A	359	HIS
1	A	464	ASN
1	A	496	HIS

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Mol	Chain	Res	Type
2	B	48	GLN
2	B	57	ASN
2	B	70	GLN
3	C	36	GLN
3	C	41	GLN
4	D	44	GLN
5	E	35	ASN
5	E	43	GLN
5	E	105	GLN
5	E	143	ASN
5	E	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	295/501 (58%)	0.05	5 (1%) 69 66	43, 60, 81, 104	0
2	B	222/236 (94%)	-0.12	4 (1%) 67 64	35, 54, 77, 90	0
3	C	212/217 (97%)	-0.17	1 (0%) 87 85	36, 57, 78, 92	0
4	D	232/464 (50%)	0.19	3 (1%) 75 72	47, 70, 97, 111	0
5	E	211/219 (96%)	0.08	3 (1%) 73 71	47, 71, 93, 106	0
All	All	1172/1637 (71%)	0.01	16 (1%) 73 71	35, 62, 90, 111	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	153	SER	4.1
5	E	7	ILE	3.9
4	D	111	PHE	3.3
2	B	149	GLY	3.2
5	E	217	GLY	3.0
1	A	296	MET	2.9
2	B	232	CYS	2.7
1	A	352	ASN	2.4
4	D	237	CYS	2.3
1	A	403	SER	2.3
1	A	402	GLY	2.2
1	A	203	TYR	2.2
2	B	132	THR	2.2
2	B	7	VAL	2.1
5	E	53	ILE	2.1
3	C	131	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.