



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:18 AM UTC

PDB ID : 6BPA / pdb_00006bpa
Title : Plasmodium vivax reticulocyte binding protein 2b (PvRBP2b) bound to monoclonal antibody 3E9
Authors : Gruszczyk, J.; Chan, L.J.; Tham, W.H.
Deposited on : 2017-11-22
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

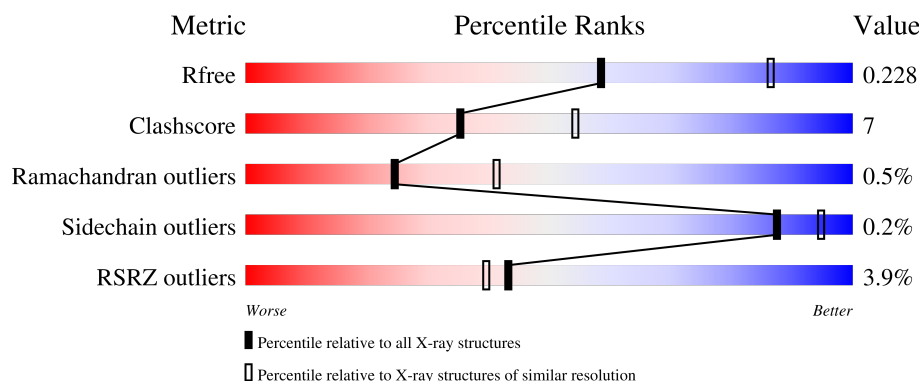
1 Overall quality at a glance

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	307	 2% 86% 10% .
1	D	307	 3% 81% 15% .
2	B	256	 3% 73% 12% 15%
2	E	256	 6% 72% 11% 16%
3	C	236	 2% 75% 14% 10%

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Mol	Chain	Length	Quality of chain
3	F	236	6% 75% 12% • 11%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12059 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 2, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2502	1603	428	462	9			
1	D	296	Total	C	N	O	S	0	0	0
			2493	1598	427	459	9			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	164	GLY	-	expression tag	UNP A5K736
A	165	ALA	-	expression tag	UNP A5K736
A	166	MET	-	expression tag	UNP A5K736
A	167	GLY	-	expression tag	UNP A5K736
A	168	SER	-	expression tag	UNP A5K736
D	164	GLY	-	expression tag	UNP A5K736
D	165	ALA	-	expression tag	UNP A5K736
D	166	MET	-	expression tag	UNP A5K736
D	167	GLY	-	expression tag	UNP A5K736
D	168	SER	-	expression tag	UNP A5K736

- Molecule 2 is a protein called Monoclonal antibody 3E9 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1628	1030	268	324	6			
2	E	215	Total	C	N	O	S	0	0	0
			1615	1022	266	322	5			

- Molecule 3 is a protein called Monoclonal antibody 3E9 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	212	Total	C	N	O	S	0	0	0
			1643	1025	270	341	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	211	Total	C	N	O	S	0	0	0
			1635	1021	268	339	7			

- Molecule 4 is BROMIDE ION (CCD ID: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Br	0	0
			1	1		

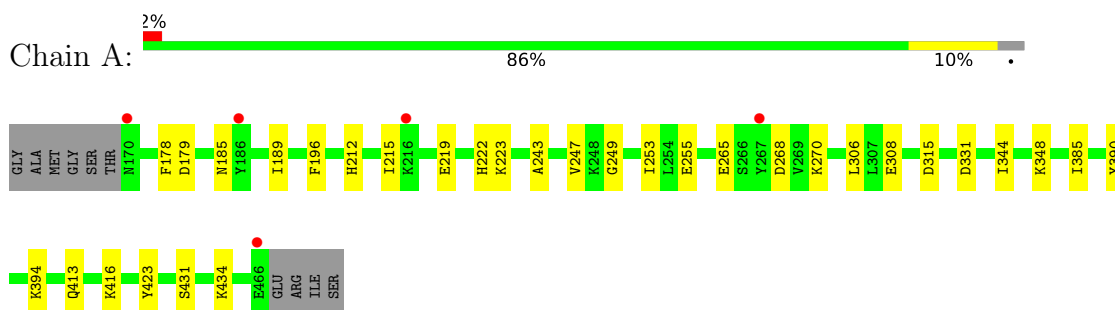
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	91	Total	O	0	0
			91	91		
5	B	121	Total	O	0	0
			121	121		
5	C	102	Total	O	0	0
			102	102		
5	D	110	Total	O	0	0
			110	110		
5	E	63	Total	O	0	0
			63	63		
5	F	55	Total	O	0	0
			55	55		

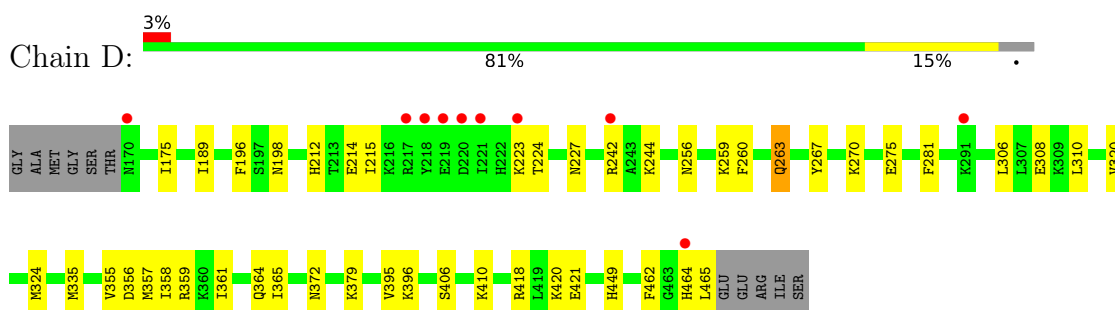
3 Residue-property plots [i](#)

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

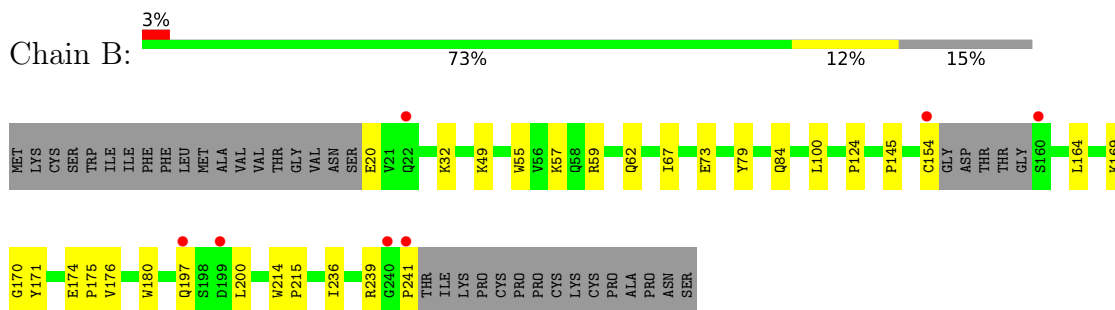
- Molecule 1: Reticulocyte binding protein 2, putative



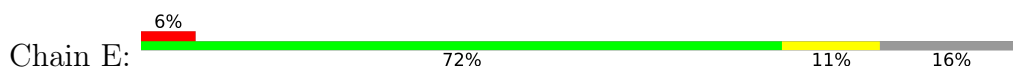
- Molecule 1: Reticulocyte binding protein 2, putative

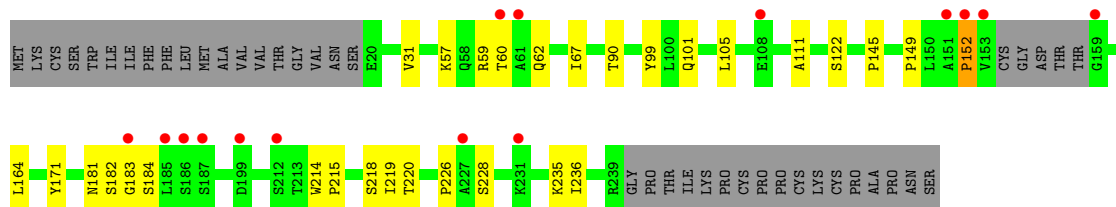


- Molecule 2: Monoclonal antibody 3E9 Fab heavy chain

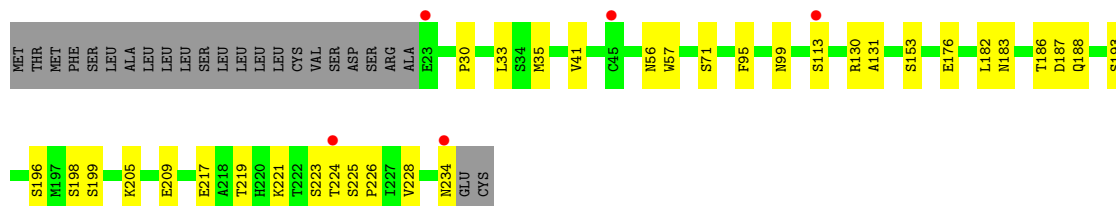
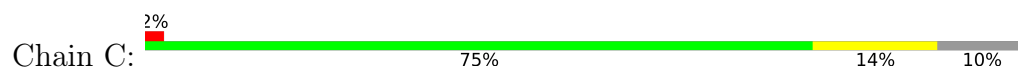


- Molecule 2: Monoclonal antibody 3E9 Fab heavy chain

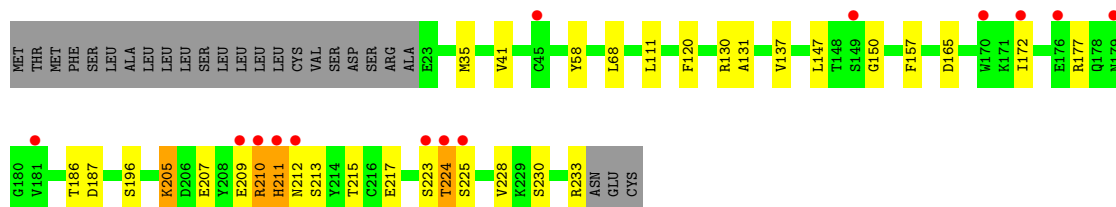
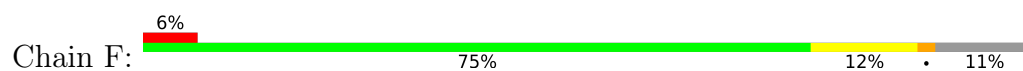




• Molecule 3: Monoclonal antibody 3E9 Fab light chain



• Molecule 3: Monoclonal antibody 3E9 Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	59.07Å 177.10Å 178.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.05 – 2.53 56.05 – 2.53	Depositor EDS
% Data completeness (in resolution range)	99.7 (56.05-2.53) 99.7 (56.05-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.55Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.194 , 0.225 0.196 , 0.228	Depositor DCC
R_{free} test set	1039 reflections (1.63%)	wwPDB-VP
Wilson B-factor (Å ²)	34.7	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12059	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% 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

Bond lengths and bond angles in the following residue types are not validated in this section: BR

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	0.15	0/2551	0.30	0/3422
1	D	0.18	0/2542	0.34	0/3410
2	B	0.17	0/1670	0.37	0/2285
2	E	0.16	0/1656	0.39	0/2265
3	C	0.18	0/1678	0.39	0/2283
3	F	0.17	0/1670	0.46	1/2272 (0.0%)
All	All	0.17	0/11767	0.37	1/15937 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	210	ARG	N-CA-C	10.90	122.73	111.07

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	2502	0	2510	24	0
1	D	2493	0	2504	34	0
2	B	1628	0	1586	22	0
2	E	1615	0	1574	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1643	0	1579	23	0
3	F	1635	0	1572	46	0
4	A	1	0	0	0	0
5	A	91	0	0	7	0
5	B	121	0	0	6	0
5	C	102	0	0	5	0
5	D	110	0	0	4	0
5	E	63	0	0	1	0
5	F	55	0	0	0	0
All	All	12059	0	11325	170	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 7.

All (170) 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)
3:F:210:ARG:HB2	3:F:211:HIS:CG	1.73	1.22
3:F:210:ARG:HB2	3:F:211:HIS:ND1	1.56	1.20
1:A:249:GLY:O	1:A:253:ILE:HD12	1.37	1.20
3:F:210:ARG:N	3:F:211:HIS:HB2	1.64	1.10
3:F:210:ARG:CA	3:F:211:HIS:HB2	1.83	1.06
3:F:207:GLU:HA	3:F:210:ARG:CZ	1.94	0.97
1:A:249:GLY:O	1:A:253:ILE:CD1	2.15	0.95
3:F:111:LEU:HD13	3:F:120:PHE:CE1	2.01	0.95
3:F:210:ARG:HB2	3:F:211:HIS:CB	1.98	0.93
3:F:210:ARG:CB	3:F:211:HIS:ND1	2.32	0.93
3:F:209:GLU:N	3:F:209:GLU:OE1	2.01	0.92
3:F:210:ARG:CB	3:F:211:HIS:HB2	2.04	0.86
2:B:84:GLN:O	5:B:301:HOH:O	1.97	0.82
3:F:210:ARG:CB	3:F:211:HIS:HD1	1.90	0.81
3:F:210:ARG:HB2	3:F:211:HIS:HB2	1.62	0.80
3:C:223:SER:O	3:C:225:SER:N	2.14	0.80
1:A:268:ASP:OD2	5:A:601:HOH:O	2.03	0.77
2:E:57:LYS:HE2	2:E:59:ARG:HD3	1.67	0.77
1:D:242:ARG:NH1	5:D:501:HOH:O	2.20	0.75
3:F:210:ARG:HB2	3:F:211:HIS:HD1	1.46	0.74
3:F:210:ARG:H	3:F:211:HIS:HB2	1.47	0.74
3:F:111:LEU:HD13	3:F:120:PHE:CZ	2.23	0.73
3:F:207:GLU:O	3:F:210:ARG:HG2	1.88	0.73
2:E:182:SER:N	2:E:183:GLY:HA2	2.05	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:ASP:OD2	5:A:602:HOH:O	2.08	0.70
3:C:176:GLU:OE2	5:C:301:HOH:O	2.09	0.70
2:E:90:THR:HG22	2:E:99:TYR:HB2	1.72	0.70
1:D:335:MET:HE2	1:D:395:VAL:HG11	1.74	0.68
3:F:186:THR:HG22	3:F:196:SER:H	1.57	0.68
3:F:210:ARG:CA	3:F:211:HIS:CB	2.69	0.68
3:C:217:GLU:HG2	3:C:228:VAL:HG22	1.74	0.68
1:D:214:GLU:HG3	1:D:310:LEU:HA	1.75	0.66
1:A:178:PHE:O	5:A:603:HOH:O	2.13	0.66
1:D:449:HIS:HD2	5:D:572:HOH:O	1.78	0.65
3:F:210:ARG:HB3	3:F:211:HIS:HD1	1.62	0.65
3:F:207:GLU:HA	3:F:210:ARG:NH2	2.11	0.65
3:F:215:THR:HG23	3:F:230:SER:HB3	1.78	0.64
2:B:154:CYS:HB2	2:B:239:ARG:HB2	1.79	0.64
3:C:56:ASN:HD22	3:C:71:SER:HA	1.62	0.64
3:F:207:GLU:HA	3:F:210:ARG:NH1	2.13	0.64
1:D:464:HIS:HB2	1:D:465:LEU:HA	1.78	0.64
3:F:147:LEU:O	3:F:205:LYS:HE2	1.97	0.64
1:A:179:ASP:OD2	5:A:604:HOH:O	2.15	0.62
3:C:234:ASN:ND2	5:C:308:HOH:O	2.27	0.62
2:B:32:LYS:HE3	5:B:335:HOH:O	1.97	0.62
3:C:153:SER:O	5:C:302:HOH:O	2.16	0.62
1:D:189:ILE:HG12	1:D:196:PHE:HE1	1.65	0.61
1:A:431:SER:OG	5:A:605:HOH:O	2.16	0.61
3:C:223:SER:O	3:C:223:SER:OG	2.18	0.60
3:F:165:ASP:OD1	3:F:165:ASP:N	2.34	0.59
3:F:111:LEU:HD13	3:F:120:PHE:CD1	2.37	0.59
1:D:223:LYS:HD3	1:D:223:LYS:C	2.27	0.59
1:A:185:ASN:O	1:A:185:ASN:ND2	2.36	0.58
3:F:111:LEU:HD12	3:F:120:PHE:CG	2.37	0.58
2:E:145:PRO:HB3	2:E:171:TYR:HB3	1.86	0.58
3:C:188:GLN:HE21	3:C:193:SER:HB3	1.69	0.58
1:D:223:LYS:O	1:D:227:ASN:HB2	2.05	0.57
3:F:223:SER:O	3:F:224:THR:HG22	2.04	0.56
2:E:101:GLN:OE1	5:E:301:HOH:O	2.18	0.56
1:A:255:GLU:OE1	5:A:606:HOH:O	2.18	0.56
1:D:308:GLU:OE1	1:D:420:LYS:NZ	2.25	0.56
2:B:241:PRO:HB2	5:B:324:HOH:O	2.07	0.55
1:D:260:PHE:O	1:D:263:GLN:NE2	2.40	0.55
3:C:30:PRO:HD2	3:C:33:LEU:HD11	1.89	0.55
1:D:244:LYS:HB2	1:D:281:PHE:CE2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:181:ASN:ND2	2:E:220:THR:H	2.05	0.55
3:C:186:THR:HG22	3:C:196:SER:H	1.71	0.54
3:F:210:ARG:CB	3:F:211:HIS:CB	2.69	0.54
2:E:181:ASN:C	2:E:183:GLY:HA2	2.32	0.54
2:E:214:TRP:CG	2:E:215:PRO:HA	2.43	0.54
2:B:145:PRO:HB3	2:B:171:TYR:HB3	1.90	0.54
3:F:111:LEU:CD1	3:F:120:PHE:CD1	2.91	0.53
3:C:99:ASN:HB2	5:C:348:HOH:O	2.07	0.53
2:E:57:LYS:CE	2:E:59:ARG:HD3	2.35	0.53
3:C:130:ARG:NH1	3:C:131:ALA:O	2.41	0.53
2:B:79:TYR:OH	5:B:302:HOH:O	2.14	0.53
3:F:223:SER:C	3:F:225:SER:H	2.17	0.52
1:D:396:LYS:HG3	2:E:122:SER:HB2	1.92	0.52
2:B:49:LYS:HG2	2:B:73:GLU:HG2	1.92	0.52
3:F:210:ARG:N	3:F:211:HIS:CB	2.56	0.52
1:D:175:ILE:HD11	1:D:244:LYS:HG3	1.92	0.52
1:A:185:ASN:HD22	1:A:185:ASN:C	2.19	0.51
1:D:215:ILE:HB	1:D:306:LEU:HD21	1.92	0.51
2:B:124:PRO:HG2	3:C:113:SER:OG	2.11	0.51
1:D:356:ASP:OD1	1:D:359:ARG:NH2	2.41	0.51
1:D:364:GLN:HB2	1:D:365:ILE:HD12	1.91	0.51
1:D:464:HIS:CB	1:D:465:LEU:HA	2.41	0.51
2:E:31:VAL:HG21	2:E:105:LEU:HD13	1.93	0.50
2:B:174:GLU:HG3	2:B:175:PRO:HA	1.93	0.50
2:B:164:LEU:HD22	2:B:236:ILE:HG21	1.94	0.50
3:C:183:ASN:ND2	3:C:199:SER:OG	2.44	0.50
3:F:111:LEU:CD1	3:F:120:PHE:CE1	2.87	0.50
2:E:226:PRO:C	2:E:228:SER:H	2.20	0.50
1:D:406:SER:O	1:D:410:LYS:NZ	2.45	0.49
3:C:219:THR:HG22	3:C:226:PRO:HB3	1.95	0.48
3:F:130:ARG:HG2	3:F:131:ALA:N	2.27	0.48
2:E:220:THR:HA	2:E:235:LYS:HA	1.95	0.48
2:E:214:TRP:CD1	2:E:215:PRO:HA	2.47	0.48
1:D:361:ILE:HG23	1:D:365:ILE:HD13	1.96	0.48
2:E:59:ARG:HG2	2:E:111:ALA:HB2	1.95	0.48
3:F:111:LEU:CD1	3:F:120:PHE:CZ	2.96	0.48
1:D:267:TYR:CZ	1:D:372:ASN:HB3	2.49	0.47
2:B:59:ARG:HB3	2:B:62:GLN:HB2	1.96	0.47
2:B:20:GLU:O	5:B:303:HOH:O	2.20	0.47
1:D:418:ARG:NH1	1:D:421:GLU:OE1	2.47	0.47
1:A:243:ALA:O	1:A:247:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:LYS:HB2	2:B:67:ILE:HD11	1.97	0.46
1:A:215:ILE:HB	1:A:306:LEU:HD21	1.97	0.46
1:A:219:GLU:O	1:A:223:LYS:HG2	2.16	0.46
1:A:315:ASP:HA	1:A:413:GLN:HB3	1.97	0.46
1:A:189:ILE:HG12	1:A:196:PHE:HE1	1.81	0.46
3:C:186:THR:HG23	3:C:187:ASP:O	2.16	0.46
3:C:205:LYS:O	3:C:209:GLU:HG2	2.16	0.46
3:F:209:GLU:HG3	3:F:233:ARG:CZ	2.46	0.46
3:C:33:LEU:HD23	3:C:35:MET:HE3	1.98	0.46
2:E:57:LYS:HB2	2:E:67:ILE:HD11	1.97	0.45
2:E:181:ASN:HD21	2:E:220:THR:H	1.64	0.45
2:E:181:ASN:HD21	2:E:219:ILE:HA	1.81	0.45
3:F:207:GLU:CA	3:F:210:ARG:NH1	2.79	0.45
1:A:212:HIS:HE1	1:A:423:TYR:OH	2.00	0.45
1:A:222:HIS:HB3	1:A:223:LYS:HZ2	1.82	0.45
1:D:357:MET:SD	1:D:361:ILE:HD12	2.57	0.45
2:B:154:CYS:O	5:B:304:HOH:O	2.21	0.44
1:D:449:HIS:CD2	5:D:572:HOH:O	2.61	0.44
3:C:35:MET:HG3	3:C:41:VAL:HG22	1.98	0.44
3:F:137:VAL:HA	3:F:157:PHE:O	2.18	0.44
1:D:212:HIS:HB2	1:D:215:ILE:HG12	2.00	0.44
2:E:60:THR:C	2:E:62:GLN:H	2.25	0.44
1:A:348:LYS:HG3	1:A:385:ILE:HG21	1.98	0.44
1:A:390:TYR:O	1:A:394:LYS:HG2	2.17	0.44
1:D:465:LEU:HA	1:D:465:LEU:HD12	1.75	0.44
3:F:217:GLU:HG2	3:F:228:VAL:HG13	1.99	0.43
2:B:197:GLN:HB3	3:C:182:LEU:HD11	2.00	0.43
2:E:181:ASN:O	2:E:184:SER:N	2.48	0.43
3:F:186:THR:HG23	3:F:187:ASP:O	2.18	0.43
1:A:265:GLU:HB2	1:A:270:LYS:HD3	2.00	0.43
1:D:263:GLN:HE21	1:D:263:GLN:HB3	1.63	0.43
1:D:189:ILE:HG12	1:D:196:PHE:CE1	2.49	0.43
3:F:58:TYR:CE1	3:F:68:LEU:HB2	2.54	0.43
2:B:214:TRP:CG	2:B:215:PRO:HA	2.54	0.43
2:B:197:GLN:O	2:B:197:GLN:HG3	2.19	0.43
1:D:320:VAL:O	1:D:324:MET:HG2	2.18	0.43
3:F:35:MET:HG3	3:F:41:VAL:HG22	2.01	0.43
3:C:221:LYS:NZ	5:C:317:HOH:O	2.50	0.42
2:E:59:ARG:HG2	2:E:111:ALA:CB	2.49	0.42
2:E:152:PRO:HD3	2:E:164:LEU:HD23	2.00	0.42
3:F:150:GLY:HA2	3:F:205:LYS:HE3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:55:TRP:CE2	2:B:100:LEU:HB2	2.54	0.42
3:C:183:ASN:HA	3:C:198:SER:O	2.19	0.42
3:C:57:TRP:CE2	3:C:95:PHE:HB2	2.54	0.42
1:D:275:GLU:OE2	1:D:379:LYS:HE3	2.20	0.42
1:D:361:ILE:HD13	1:D:462:PHE:HZ	1.84	0.42
2:B:170:GLY:HA2	2:B:200:LEU:HB3	2.02	0.42
1:D:270:LYS:HD2	1:D:270:LYS:HA	1.83	0.42
3:F:209:GLU:N	3:F:209:GLU:CD	2.73	0.42
2:B:79:TYR:HB2	2:B:84:GLN:HG2	2.01	0.42
2:B:180:TRP:HZ3	2:B:236:ILE:HD13	1.85	0.42
1:A:222:HIS:HB3	1:A:223:LYS:NZ	2.35	0.41
1:D:198:ASN:ND2	5:D:505:HOH:O	2.33	0.41
1:A:308:GLU:HA	1:A:416:LYS:HD3	2.01	0.41
3:F:212:ASN:OD1	3:F:213:SER:N	2.53	0.41
1:A:344:ILE:O	1:A:348:LYS:HB2	2.20	0.41
1:D:355:VAL:O	1:D:358:ILE:HG22	2.20	0.41
2:B:169:LYS:HE2	2:B:169:LYS:HB3	1.82	0.41
3:F:111:LEU:CD1	3:F:120:PHE:CG	3.03	0.41
1:D:256:ASN:HB3	1:D:259:LYS:HB2	2.03	0.40
1:A:434:LYS:NZ	5:A:621:HOH:O	2.54	0.40
2:E:181:ASN:C	2:E:184:SER:H	2.29	0.40
3:F:172:ILE:HD12	3:F:177:ARG:HD3	2.03	0.40
2:E:149:PRO:CB	2:E:236:ILE:HD12	2.51	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	295/307 (96%)	290 (98%)	5 (2%)	0	100	100
1	D	294/307 (96%)	286 (97%)	7 (2%)	1 (0%)	36	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	213/256 (83%)	209 (98%)	4 (2%)	0	100	100
2	E	211/256 (82%)	203 (96%)	6 (3%)	2 (1%)	14	26
3	C	210/236 (89%)	203 (97%)	6 (3%)	1 (0%)	24	41
3	F	209/236 (89%)	199 (95%)	7 (3%)	3 (1%)	9	16
All	All	1432/1598 (90%)	1390 (97%)	35 (2%)	7 (0%)	24	41

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	224	THR
3	F	211	HIS
3	F	205	LYS
2	E	218	SER
3	F	224	THR
1	D	224	THR
2	E	152	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	A	279/286 (98%)	279 (100%)	0	100	100
1	D	278/286 (97%)	277 (100%)	1 (0%)	84	92
2	B	184/218 (84%)	183 (100%)	1 (0%)	81	91
2	E	182/218 (84%)	182 (100%)	0	100	100
3	C	191/213 (90%)	191 (100%)	0	100	100
3	F	190/213 (89%)	190 (100%)	0	100	100
All	All	1304/1434 (91%)	1302 (100%)	2 (0%)	87	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	176	VAL
1	D	263	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	212	HIS
1	A	252	ASN
3	C	56	ASN
3	C	159	ASN
3	C	183	ASN
3	C	188	GLN
1	D	317	GLN
1	D	391	HIS
1	D	413	GLN
1	D	444	ASN
1	D	449	HIS
2	E	58	GLN
2	E	181	ASN
2	E	190	HIS
3	F	159	ASN
3	F	160	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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	297/307 (96%)	0.02	5 (1%) 69 66	22, 42, 70, 94	0
1	D	296/307 (96%)	0.03	10 (3%) 48 44	23, 39, 64, 102	0
2	B	217/256 (84%)	-0.15	7 (3%) 50 47	19, 31, 54, 82	0
2	E	215/256 (83%)	0.53	15 (6%) 22 20	24, 53, 88, 103	0
3	C	212/236 (89%)	-0.17	5 (2%) 59 56	22, 36, 57, 65	0
3	F	211/236 (89%)	0.40	14 (6%) 24 22	27, 52, 90, 111	0
All	All	1448/1598 (90%)	0.10	56 (3%) 43 39	19, 40, 78, 111	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	153	VAL	6.4
2	B	241	PRO	5.3
3	F	172	ILE	4.6
3	F	210	ARG	4.3
3	F	211	HIS	4.1
2	E	152	PRO	4.0
2	B	154	CYS	3.8
1	D	464	HIS	3.6
3	F	176	GLU	3.3
1	D	219	GLU	3.2
1	A	170	ASN	3.1
2	E	227	ALA	3.0
2	E	60	THR	3.0
2	E	183	GLY	2.9
2	B	240	GLY	2.9
2	E	199	ASP	2.9
3	F	224	THR	2.8
2	B	199	ASP	2.8
2	E	159	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
3	F	223	SER	2.8
2	E	212	SER	2.8
3	F	212	ASN	2.8
2	E	151	ALA	2.8
1	D	170	ASN	2.6
1	A	466	GLU	2.6
2	E	61	ALA	2.6
3	F	179	ASN	2.6
2	E	231	LYS	2.5
3	C	23	GLU	2.5
2	E	108	GLU	2.4
3	C	113	SER	2.4
1	A	267	TYR	2.4
3	C	224	THR	2.4
2	E	186	SER	2.3
1	D	218	TYR	2.3
2	E	187	SER	2.3
3	F	225	SER	2.3
3	C	45	CYS	2.3
3	F	209	GLU	2.3
1	D	220	ASP	2.3
2	B	160	SER	2.2
3	C	234	ASN	2.2
1	A	186	TYR	2.2
2	E	185	LEU	2.2
1	D	221	ILE	2.2
1	D	223	LYS	2.2
3	F	149	SER	2.2
1	D	217	ARG	2.2
1	D	242	ARG	2.2
3	F	181	VAL	2.1
3	F	45	CYS	2.1
3	F	170	TRP	2.1
1	D	291	LYS	2.1
2	B	22	GLN	2.1
1	A	216	LYS	2.0
2	B	197	GLN	2.0

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	BR	A	501	1/1	0.99	0.06	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.