



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 04:00 PM UTC

PDB ID : 4YBQ / pdb_00004ybq
Title : Rat GLUT5 with Fv in the outward-open form
Authors : Nomura, N.; Shimamura, T.; Iwata, S.
Deposited on : 2015-02-19
Resolution : 3.27 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

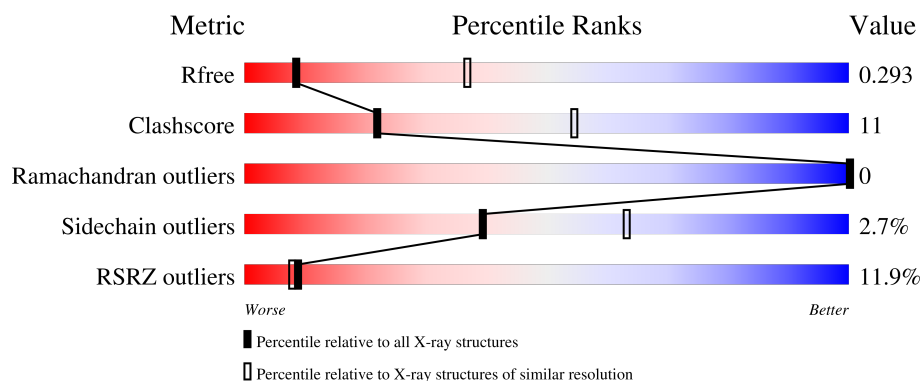
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.27 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	1303 (3.30-3.26)
Clashscore	190562	1354 (3.30-3.26)
Ramachandran outliers	187476	1334 (3.30-3.26)
Sidechain outliers	187428	1333 (3.30-3.26)
RSRZ outliers	180081	1303 (3.30-3.26)

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	508	10% 61% 27% • 11%
1	B	508	12% 64% 25% • 9%
2	C	122	11% 81% 12% • 6%
2	E	122	14% 76% 17% • 6%
3	D	136	14% 72% 15% • 12%

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Mol	Chain	Length	Quality of chain
3	F	136	4% 67% 19% • 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10657 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 Solute carrier family 2, facilitated glucose transporter member 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	0	0
			3486	2313	553	601	19			
1	B	462	Total	C	N	O	S	0	0	0
			3567	2361	567	620	19			

There are 14 discrepancies between the modelled and reference sequences:

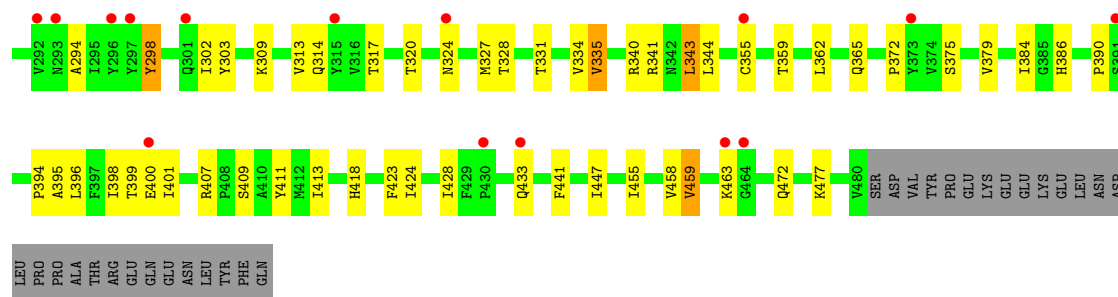
Chain	Residue	Modelled	Actual	Comment	Reference
A	50	TYR	ASN	engineered mutation	UNP P43427
A	503	GLU	-	expression tag	UNP P43427
A	504	ASN	-	expression tag	UNP P43427
A	505	LEU	-	expression tag	UNP P43427
A	506	TYR	-	expression tag	UNP P43427
A	507	PHE	-	expression tag	UNP P43427
A	508	GLN	-	expression tag	UNP P43427
B	50	TYR	ASN	engineered mutation	UNP P43427
B	503	GLU	-	expression tag	UNP P43427
B	504	ASN	-	expression tag	UNP P43427
B	505	LEU	-	expression tag	UNP P43427
B	506	TYR	-	expression tag	UNP P43427
B	507	PHE	-	expression tag	UNP P43427
B	508	GLN	-	expression tag	UNP P43427

- Molecule 2 is a protein called antibody Fv fragment light chain.

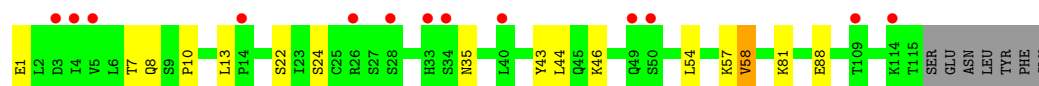
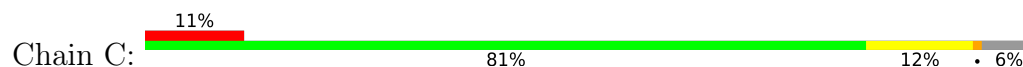
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	115	Total	C	N	O	S	0	0	0
			885	562	147	174	2			
2	E	115	Total	C	N	O	S	0	0	0
			885	562	147	174	2			

- Molecule 3 is a protein called antibody Fv fragment heavy chain.

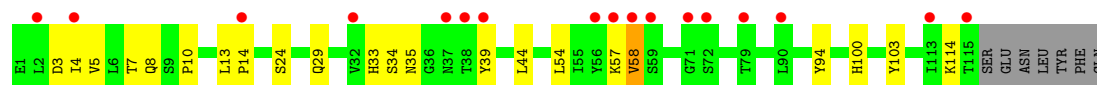
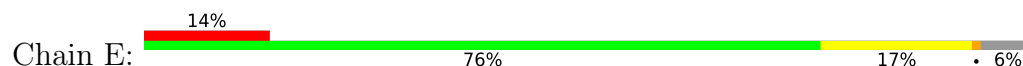
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	120	Total	C	N	O	S	0	0	0
			921	577	160	180	4			
3	F	119	Total	C	N	O	S	0	0	0
			913	571	159	179	4			



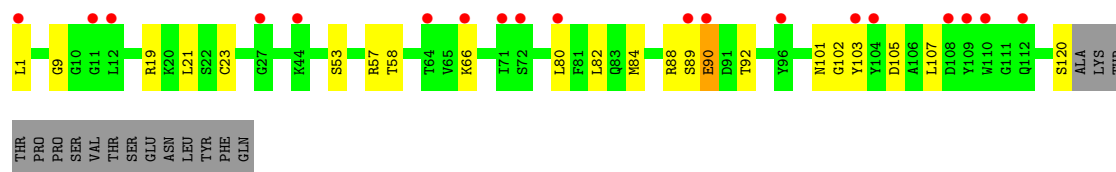
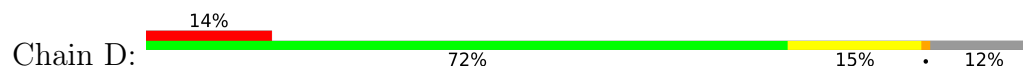
- Molecule 2: antibody Fv fragment light chain



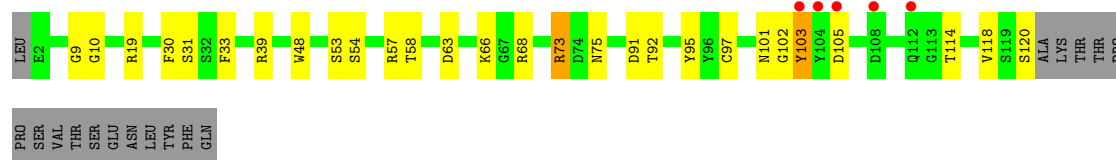
- Molecule 2: antibody Fv fragment light chain



- Molecule 3: antibody Fv fragment heavy chain



- Molecule 3: antibody Fv fragment heavy chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.77Å 151.54Å 106.40Å 90.00° 97.25° 90.00°	Depositor
Resolution (Å)	36.49 – 3.27 36.49 – 3.27	Depositor EDS
% Data completeness (in resolution range)	99.8 (36.49-3.27) 91.6 (36.49-3.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.242 , 0.288 0.253 , 0.293	Depositor DCC
R_{free} test set	1877 reflections (3.77%)	wwPDB-VP
Wilson B-factor (Å ²)	106.3	Xtriage
Anisotropy	0.352	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 78.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	10657	wwPDB-VP
Average B, all atoms (Å ²)	157.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.06% 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	0.38	0/3564	0.86	2/4845 (0.0%)
1	B	0.38	0/3647	0.86	4/4957 (0.1%)
2	C	0.35	0/905	0.78	0/1226
2	E	0.37	0/905	0.84	2/1226 (0.2%)
3	D	0.32	0/942	0.84	1/1275 (0.1%)
3	F	0.34	0/934	0.89	1/1264 (0.1%)
All	All	0.37	0/10897	0.85	10/14793 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	SER	CA-C-N	6.54	126.17	119.56
1	B	40	SER	C-N-CA	6.54	126.17	119.56
2	E	5	VAL	N-CA-C	5.79	116.64	108.36
3	D	102	GLY	N-CA-C	5.56	120.89	114.16
3	F	102	GLY	N-CA-C	5.56	120.88	114.16
1	A	437	GLY	CA-C-N	5.28	124.79	119.19
1	A	437	GLY	C-N-CA	5.28	124.79	119.19
1	B	459	VAL	CA-C-N	5.25	125.46	120.31
1	B	459	VAL	C-N-CA	5.25	125.46	120.31
2	E	3	ASP	N-CA-C	5.22	117.91	107.62

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	3486	0	3646	96	0
1	B	3567	0	3715	93	0
2	C	885	0	871	11	0
2	E	885	0	871	13	0
3	D	921	0	880	16	0
3	F	913	0	866	21	0
All	All	10657	0	10849	229	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 11.

All (229) 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:A:364:LEU:HB3	1:A:371:MET:HG3	1.70	0.74
1:B:38:VAL:O	1:B:131:ARG:NH2	2.22	0.72
1:B:7:GLU:OE1	1:B:155:LYS:NZ	2.22	0.71
1:A:25:PHE:O	1:A:29:PHE:HB3	1.90	0.71
2:E:14:PRO:HB2	2:E:114:LYS:HG2	1.72	0.71
1:B:458:VAL:O	1:B:477:LYS:NZ	2.23	0.71
3:F:92:THR:HG22	3:F:118:VAL:H	1.53	0.70
1:B:37:ALA:O	1:B:40:SER:OG	2.10	0.70
1:A:289:LEU:HB3	1:A:447:ILE:HD13	1.73	0.70
1:A:26:GLY:HA2	1:A:201:PRO:HB2	1.74	0.70
1:B:289:LEU:HB3	1:B:447:ILE:HD13	1.74	0.69
1:B:344:LEU:HB3	1:B:455:ILE:HD13	1.75	0.69
1:B:303:TYR:HB3	1:B:313:VAL:HG22	1.75	0.68
1:B:25:PHE:O	1:B:29:PHE:HB3	1.94	0.67
1:B:154:PRO:O	1:B:158:ARG:N	2.27	0.67
1:A:20:THR:HG21	1:A:161:LEU:HD22	1.76	0.67
1:B:294:ALA:O	1:B:298:TYR:HB3	1.95	0.67
3:F:68:ARG:NH2	3:F:91:ASP:OD2	2.29	0.65
1:B:98:LYS:HE2	1:B:214:GLU:HG2	1.80	0.62
1:B:276:GLN:HB3	1:B:401:ILE:HG21	1.83	0.61
1:A:154:PRO:O	1:A:158:ARG:N	2.34	0.61
1:A:358:LEU:HG	1:A:378:CYS:SG	2.41	0.61
1:B:156:ASN:OD1	1:B:156:ASN:N	2.34	0.60
1:A:344:LEU:HB3	1:A:455:ILE:HD13	1.83	0.59
1:A:76:MET:HG3	1:A:128:ILE:HG23	1.84	0.59
2:C:44:LEU:HB2	2:C:54:LEU:HD11	1.84	0.59
1:A:341:ARG:NH1	1:A:459:VAL:O	2.34	0.59
1:A:246:MET:SD	3:F:57:ARG:NH2	2.76	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:ALA:O	1:B:41:PRO:HD3	2.03	0.58
1:A:153:ALA:HB2	1:A:161:LEU:HD12	1.86	0.58
1:A:327:MET:O	1:A:331:THR:OG1	2.11	0.58
1:A:368:ILE:HG22	1:A:370:TRP:H	1.68	0.58
1:B:76:MET:HG3	1:B:128:ILE:HG23	1.86	0.58
3:F:73:ARG:NE	3:F:75:ASN:OD1	2.37	0.57
3:F:30:PHE:O	3:F:73:ARG:NH2	2.37	0.57
1:B:298:TYR:CZ	1:B:302:ILE:HD11	2.39	0.57
3:D:53:SER:HB3	3:D:58:THR:HB	1.87	0.57
1:B:365:GLN:HB2	1:B:372:PRO:HD3	1.86	0.57
3:D:21:LEU:HD11	3:D:84:MET:HE2	1.87	0.56
1:A:230:GLU:OE1	3:F:57:ARG:NH1	2.39	0.56
1:B:75:SER:HB3	1:B:423:PHE:HE1	1.71	0.56
1:A:272:SER:O	1:A:478:ASN:ND2	2.39	0.56
1:B:73:THR:HG22	1:B:128:ILE:HG12	1.87	0.55
1:A:38:VAL:O	1:A:131:ARG:NH2	2.35	0.55
1:A:214:GLU:OE1	1:A:215:SER:N	2.36	0.55
1:A:276:GLN:HB3	1:A:401:ILE:HG21	1.89	0.55
1:A:191:TRP:H	1:A:191:TRP:CD1	2.25	0.54
1:A:311:ASN:OD1	1:A:312:ASP:N	2.40	0.54
1:A:334:VAL:HG12	1:A:343:LEU:HD11	1.89	0.54
1:A:240:LYS:HG3	3:F:105:ASP:CG	2.33	0.54
1:B:394:PRO:O	1:B:398:ILE:HG13	2.08	0.54
2:E:44:LEU:HB2	2:E:54:LEU:HD11	1.90	0.54
1:B:123:SER:OG	1:B:126:ILE:HG12	2.07	0.53
1:A:313:VAL:HA	1:A:316:VAL:HG22	1.90	0.53
1:A:104:ASN:HD21	1:A:141:SER:HB3	1.74	0.53
1:B:20:THR:HG21	1:B:161:LEU:HD22	1.91	0.52
1:B:334:VAL:HG12	1:B:343:LEU:HD11	1.92	0.52
2:E:57:LYS:O	2:E:58:VAL:HG22	2.09	0.52
1:A:103:PHE:HA	1:A:106:ILE:HG22	1.92	0.52
1:B:24:ALA:O	1:B:28:SER:OG	2.21	0.52
1:A:309:LYS:O	1:A:313:VAL:HG13	2.10	0.51
1:A:394:PRO:O	1:A:398:ILE:HG13	2.10	0.51
2:C:57:LYS:O	2:C:58:VAL:HG22	2.09	0.51
1:A:364:LEU:CB	1:A:371:MET:HG3	2.39	0.51
2:C:7:THR:OG1	2:E:7:THR:HG21	2.10	0.51
1:A:8:LYS:HG3	3:F:103:TYR:CE1	2.45	0.51
1:A:117:CYS:O	1:A:121:ALA:N	2.30	0.51
1:B:97:ARG:NH1	1:B:151:GLU:OE2	2.43	0.51
1:B:238:GLY:C	2:C:35:ASN:HD21	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:MET:O	1:B:331:THR:OG1	2.15	0.51
1:A:70:TRP:HA	1:A:70:TRP:CE3	2.46	0.51
1:B:159:GLY:HA2	1:B:396:LEU:HD21	1.93	0.50
1:B:154:PRO:HG2	1:B:157:LEU:HB2	1.93	0.50
1:B:372:PRO:O	1:B:375:SER:OG	2.23	0.50
3:F:53:SER:HB3	3:F:58:THR:HB	1.93	0.50
1:A:331:THR:HG21	1:A:392:PRO:HG3	1.94	0.49
1:B:103:PHE:HA	1:B:106:ILE:HG22	1.94	0.49
1:B:151:GLU:OE2	1:B:407:ARG:NH1	2.44	0.49
1:B:359:THR:HG22	1:B:441:PHE:HB2	1.94	0.49
3:D:89:SER:O	3:D:92:THR:HG22	2.12	0.49
1:B:303:TYR:HD2	1:B:313:VAL:HG13	1.78	0.49
1:A:266:LYS:O	1:A:270:MET:HG3	2.13	0.49
2:C:1:GLU:OE2	3:D:66:LYS:NZ	2.32	0.49
1:A:347:GLY:HA3	1:A:390:PRO:HD3	1.93	0.49
1:B:104:ASN:HD21	1:B:141:SER:HB3	1.78	0.48
1:B:302:ILE:CD1	1:B:379:VAL:HG21	2.43	0.48
1:B:303:TYR:CD2	1:B:313:VAL:HG13	2.48	0.48
1:B:150:GLY:HA3	1:B:399:THR:HG21	1.94	0.48
1:B:386:HIS:HA	1:B:390:PRO:HD2	1.95	0.48
1:A:166:GLN:HA	1:A:169:ILE:HD12	1.95	0.48
1:A:327:MET:HE2	1:A:384:ILE:HG23	1.95	0.48
1:A:354:ALA:O	1:A:358:LEU:HB2	2.13	0.48
1:B:76:MET:HE3	1:B:132:LEU:HD13	1.96	0.48
3:D:23:CYS:HB3	3:D:80:LEU:HB3	1.95	0.48
2:E:8:GLN:OE1	2:E:94:TYR:HA	2.13	0.48
1:B:341:ARG:NH1	1:B:459:VAL:O	2.45	0.48
1:B:235:THR:HA	2:C:35:ASN:OD1	2.13	0.48
1:A:151:GLU:OE2	1:A:407:ARG:NH1	2.47	0.48
2:E:4:ILE:HG13	2:E:100:HIS:HB2	1.96	0.48
1:B:340:ARG:NH1	1:B:400:GLU:OE2	2.47	0.47
1:A:424:ILE:HG23	1:A:428:ILE:HD12	1.95	0.47
1:B:240:LYS:HG3	3:D:105:ASP:OD2	2.13	0.47
1:B:309:LYS:O	1:B:313:VAL:HG23	2.14	0.47
2:C:22:SER:OG	2:C:81:LYS:HG2	2.14	0.47
1:A:70:TRP:HA	1:A:70:TRP:HE3	1.78	0.47
1:B:264:VAL:HG13	1:B:413:ILE:HD11	1.95	0.47
1:B:424:ILE:HG23	1:B:428:ILE:HD12	1.96	0.47
1:A:310:SER:O	1:A:313:VAL:HG22	2.15	0.47
1:A:386:HIS:HA	1:A:390:PRO:HD2	1.97	0.47
1:A:300:ASP:OD1	1:A:301:GLN:N	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ALA:HB2	1:A:376:ILE:HD11	1.97	0.46
1:B:298:TYR:OH	1:B:362:LEU:HD11	2.14	0.46
1:A:461:GLU:HG3	1:A:463:LYS:HG2	1.97	0.46
1:A:191:TRP:CD1	1:A:191:TRP:N	2.83	0.46
1:A:93:ASN:OD1	1:A:222:GLN:NE2	2.48	0.46
1:B:98:LYS:O	1:B:102:LEU:HG	2.16	0.46
1:B:153:ALA:HB2	1:B:161:LEU:HD12	1.97	0.46
1:A:123:SER:OG	1:A:126:ILE:HG12	2.15	0.46
3:D:21:LEU:HD13	3:D:82:LEU:HD23	1.98	0.46
1:A:277:LEU:HD11	1:A:413:ILE:HG21	1.98	0.46
1:A:309:LYS:O	1:A:313:VAL:N	2.43	0.46
1:A:306:ALA:HB3	1:A:308:VAL:HG23	1.97	0.45
1:B:267:LEU:HD12	1:B:409:SER:HB2	1.98	0.45
1:B:284:MET:HE3	1:B:418:HIS:HB2	1.98	0.45
2:C:46:LYS:NZ	2:C:88:GLU:O	2.36	0.45
3:F:39:ARG:HD3	3:F:95:TYR:CZ	2.51	0.45
1:A:237:ARG:NH2	1:A:245:GLU:OE2	2.50	0.45
1:B:253:ASP:O	1:B:257:LYS:HB2	2.16	0.45
1:A:22:LEU:HD21	1:A:208:LEU:HD12	1.97	0.45
1:A:30:GLN:HE22	1:A:202:ALA:HB2	1.82	0.45
1:A:299:ALA:O	1:A:302:ILE:HG22	2.16	0.45
1:B:75:SER:HB3	1:B:423:PHE:CE1	2.51	0.45
2:E:33:HIS:CD2	2:E:34:SER:H	2.34	0.45
1:B:34:ASN:O	1:B:38:VAL:HG23	2.15	0.45
1:B:41:PRO:O	1:B:44:PHE:HB2	2.17	0.45
1:B:214:GLU:OE1	1:B:215:SER:N	2.37	0.45
1:B:327:MET:HE2	1:B:384:ILE:HG23	1.97	0.45
1:A:217:ARG:NH1	1:A:249:ILE:HG12	2.32	0.45
1:A:98:LYS:HB3	1:A:98:LYS:HE2	1.66	0.44
1:A:167:LEU:O	1:A:171:VAL:HG23	2.16	0.44
1:A:335:VAL:HG23	1:A:343:LEU:HD12	1.99	0.44
1:B:77:PHE:HB3	1:B:78:PRO:HD3	1.98	0.44
3:D:9:GLY:O	3:D:19:ARG:HD2	2.18	0.44
3:F:10:GLY:H	3:F:114:THR:HG21	1.83	0.44
1:A:295:ILE:HG13	1:A:382:TYR:CE2	2.53	0.44
1:B:29:PHE:CE2	1:B:172:GLY:HA2	2.52	0.44
1:A:284:MET:HE3	1:A:418:HIS:HB2	2.00	0.44
1:B:355:CYS:O	1:B:359:THR:HG23	2.18	0.44
2:E:103:TYR:HB2	3:F:48:TRP:CD2	2.51	0.43
1:B:314:GLN:O	1:B:317:THR:OG1	2.27	0.43
1:A:104:ASN:ND2	1:A:141:SER:HB3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:LYS:O	1:A:158:ARG:HB3	2.18	0.43
1:B:38:VAL:O	1:B:41:PRO:HD2	2.19	0.43
1:A:98:LYS:O	1:A:102:LEU:HG	2.18	0.43
1:A:359:THR:HG21	1:A:442:ILE:HG13	2.00	0.43
1:B:280:THR:HG22	1:B:398:ILE:HG12	2.00	0.43
1:A:256:GLU:OE1	1:A:405:SER:OG	2.36	0.43
1:B:395:ALA:O	1:B:411:TYR:OH	2.36	0.43
3:F:63:ASP:O	3:F:66:LYS:HG2	2.19	0.43
1:A:29:PHE:CE2	1:A:172:GLY:HA2	2.54	0.43
1:B:221:ILE:HG23	1:B:253:ASP:OD1	2.18	0.43
1:B:240:LYS:HG3	3:D:105:ASP:CG	2.44	0.43
1:A:238:GLY:C	2:E:35:ASN:HD21	2.27	0.43
1:A:169:ILE:O	1:A:173:ILE:HG13	2.19	0.43
1:A:262:ILE:HD13	1:A:406:SER:HB3	2.00	0.43
1:B:115:MET:O	1:B:119:LYS:HG2	2.19	0.43
1:A:7:GLU:OE1	1:A:7:GLU:N	2.51	0.42
1:B:230:GLU:OE2	3:D:57:ARG:NH1	2.52	0.42
1:B:259:ALA:O	1:B:266:LYS:NZ	2.40	0.42
2:E:8:GLN:HA	2:E:24:SER:O	2.19	0.42
1:A:240:LYS:HG3	3:F:105:ASP:OD2	2.19	0.42
1:A:235:THR:HA	2:E:35:ASN:OD1	2.19	0.42
1:B:257:LYS:HD2	1:B:257:LYS:HA	1.83	0.42
3:D:101:ASN:O	3:D:105:ASP:N	2.53	0.42
3:F:33:PHE:O	3:F:73:ARG:NH2	2.44	0.42
1:A:108:SER:O	1:A:111:PRO:HD2	2.20	0.42
1:B:267:LEU:HD22	1:B:277:LEU:HD21	2.02	0.42
2:E:10:PRO:HG3	2:E:13:LEU:HD13	2.01	0.42
1:A:276:GLN:HB3	1:A:401:ILE:CG2	2.50	0.42
3:F:68:ARG:HH22	3:F:91:ASP:CG	2.24	0.42
1:B:10:GLY:HA2	1:B:239:TRP:CH2	2.55	0.41
1:B:79:PHE:CE2	1:B:83:ILE:HD11	2.55	0.41
1:B:169:ILE:O	1:B:173:ILE:HG13	2.20	0.41
1:B:324:ASN:O	1:B:328:THR:OG1	2.20	0.41
2:C:8:GLN:HA	2:C:24:SER:O	2.20	0.41
1:A:148:TYR:O	1:A:152:LEU:HB2	2.20	0.41
1:A:247:GLU:O	1:A:251:LYS:HG2	2.20	0.41
1:B:167:LEU:O	1:B:171:VAL:HG23	2.20	0.41
1:B:298:TYR:CE2	1:B:302:ILE:HD11	2.56	0.41
1:A:335:VAL:HG13	1:A:340:ARG:HH11	1.85	0.41
2:C:10:PRO:HG2	2:C:13:LEU:HD13	2.03	0.41
2:C:43:TYR:HE2	3:D:107:LEU:O	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:VAL:O	1:B:167:LEU:HB3	2.21	0.41
3:F:101:ASN:O	3:F:105:ASP:N	2.53	0.41
1:A:97:ARG:HB3	1:A:148:TYR:HB2	2.02	0.41
1:A:159:GLY:O	1:A:163:VAL:HG23	2.20	0.41
1:B:190:GLY:HA3	1:B:194:LEU:HD13	2.02	0.41
1:B:309:LYS:O	1:B:313:VAL:N	2.47	0.41
1:B:317:THR:O	1:B:320:THR:OG1	2.31	0.41
1:A:30:GLN:O	1:A:34:ASN:HB2	2.21	0.41
1:A:165:PRO:O	1:A:169:ILE:HG13	2.21	0.41
1:A:264:VAL:HG13	1:A:413:ILE:HD11	2.03	0.41
1:A:324:ASN:O	1:A:328:THR:OG1	2.16	0.41
1:B:240:LYS:HE2	3:D:105:ASP:HB3	2.03	0.41
1:A:31:TYR:O	1:A:35:VAL:HG23	2.20	0.41
1:A:310:SER:HA	1:A:313:VAL:HG22	2.02	0.41
1:B:463:LYS:HB2	1:B:463:LYS:HE3	1.88	0.41
3:D:88:ARG:HB2	3:D:90:GLU:HG2	2.03	0.41
1:A:451:THR:O	1:A:455:ILE:HG13	2.21	0.41
1:B:8:LYS:HG3	3:D:103:TYR:HE1	1.86	0.41
1:B:30:GLN:NE2	1:B:198:THR:O	2.54	0.41
1:B:217:ARG:NH1	1:B:249:ILE:HG12	2.35	0.41
1:B:335:VAL:HG23	1:B:343:LEU:HD12	2.03	0.41
3:F:9:GLY:O	3:F:19:ARG:HD2	2.20	0.41
3:F:31:SER:O	3:F:54:SER:HB2	2.21	0.41
1:A:245:GLU:O	1:A:249:ILE:HG13	2.21	0.41
1:A:375:SER:O	1:A:379:VAL:HG23	2.20	0.41
1:B:10:GLY:HA2	1:B:239:TRP:HH2	1.85	0.41
1:A:331:THR:O	1:A:335:VAL:HB	2.21	0.40
1:A:361:ALA:HB1	1:A:375:SER:OG	2.21	0.40
1:A:399:THR:HG23	1:A:407:ARG:HD3	2.04	0.40
1:B:250:ARG:HH22	3:D:57:ARG:HD3	1.86	0.40
1:A:268:PHE:CE1	1:A:277:LEU:HD21	2.56	0.40
1:B:284:MET:SD	1:B:394:PRO:HB2	2.62	0.40
1:A:230:GLU:HG3	3:F:57:ARG:HH22	1.86	0.40
1:B:226:GLU:OE2	1:B:250:ARG:NH2	2.54	0.40
1:A:190:GLY:HA3	1:A:194:LEU:HD13	2.03	0.40
1:B:84:GLY:O	1:B:88:VAL:HG23	2.21	0.40
2:E:39:TYR:CE1	3:F:105:ASP:HB2	2.56	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	448/508 (88%)	436 (97%)	12 (3%)	0	100	100
1	B	458/508 (90%)	447 (98%)	11 (2%)	0	100	100
2	C	113/122 (93%)	110 (97%)	3 (3%)	0	100	100
2	E	113/122 (93%)	110 (97%)	3 (3%)	0	100	100
3	D	118/136 (87%)	117 (99%)	1 (1%)	0	100	100
3	F	117/136 (86%)	116 (99%)	1 (1%)	0	100	100
All	All	1367/1532 (89%)	1336 (98%)	31 (2%)	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	378/433 (87%)	366 (97%)	12 (3%)	34	60
1	B	388/433 (90%)	379 (98%)	9 (2%)	44	66
2	C	101/108 (94%)	100 (99%)	1 (1%)	68	77
2	E	101/108 (94%)	99 (98%)	2 (2%)	48	68
3	D	98/113 (87%)	95 (97%)	3 (3%)	35	61
3	F	97/113 (86%)	93 (96%)	4 (4%)	27	55
All	All	1163/1308 (89%)	1132 (97%)	31 (3%)	39	63

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	TRP
1	A	156	ASN
1	A	174	LEU
1	A	191	TRP
1	A	301	GLN
1	A	314	GLN
1	A	335	VAL
1	A	343	LEU
1	A	358	LEU
1	A	378	CYS
1	A	396	LEU
1	A	433	GLN
1	B	156	ASN
1	B	174	LEU
1	B	241	ASP
1	B	267	LEU
1	B	298	TYR
1	B	335	VAL
1	B	343	LEU
1	B	433	GLN
1	B	472	GLN
2	C	58	VAL
3	D	1	LEU
3	D	90	GLU
3	D	120	SER
2	E	29	GLN
2	E	58	VAL
3	F	73	ARG
3	F	97	CYS
3	F	103	TYR
3	F	120	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	104	ASN
1	A	205	GLN
1	A	288	GLN
1	A	342	ASN
1	A	471	ASN

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Mol	Chain	Res	Type
1	B	143	ASN
1	B	222	GLN
1	B	271	GLN
1	B	288	GLN
1	B	365	GLN
1	B	433	GLN
2	E	33	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	452/508 (88%)	0.58	52 (11%) 9 8	77, 135, 291, 452	0
1	B	462/508 (90%)	0.67	59 (12%) 7 6	78, 137, 297, 455	0
2	C	115/122 (94%)	0.58	13 (11%) 10 9	91, 127, 188, 232	0
2	E	115/122 (94%)	0.74	17 (14%) 5 5	100, 135, 193, 233	0
3	D	120/136 (88%)	0.84	19 (15%) 5 4	94, 156, 261, 285	0
3	F	119/136 (87%)	0.33	5 (4%) 40 26	94, 159, 264, 286	0
All	All	1383/1532 (90%)	0.62	165 (11%) 9 8	77, 139, 281, 455	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	9	THR	13.8
3	D	103	TYR	8.9
1	A	435	GLY	8.3
1	A	422	ASN	7.3
2	E	57	LYS	6.9
1	B	258	ALA	6.7
1	A	296	TYR	6.2
1	A	259	ALA	6.0
1	B	259	ALA	6.0
2	E	37	ASN	5.6
1	A	260	GLY	5.6
1	B	190	GLY	5.5
2	E	38	THR	5.0
3	F	103	TYR	4.9
2	C	14	PRO	4.9
1	B	8	LYS	4.8
1	A	288	GLN	4.8
3	D	110	TRP	4.8
1	A	436	LEU	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	258	ALA	4.7
1	B	293	ASN	4.7
1	A	206	LEU	4.7
1	B	103	PHE	4.7
3	D	112	GLN	4.6
1	B	155	LYS	4.3
1	B	184	VAL	4.3
1	B	297	TYR	4.2
2	E	59	SER	4.2
1	B	157	LEU	4.2
2	E	2	LEU	4.2
2	C	34	SER	4.1
3	F	104	TYR	4.1
1	A	7	GLU	4.1
2	C	5	VAL	3.9
1	B	95	LEU	3.9
1	A	262	ILE	3.9
3	D	96	TYR	3.9
1	A	211	PHE	3.8
1	B	181	LEU	3.8
2	E	39	TYR	3.7
1	B	196	GLY	3.7
1	A	293	ASN	3.6
1	B	464	GLY	3.6
1	A	38	VAL	3.6
1	A	36	ALA	3.6
1	A	95	LEU	3.6
3	D	108	ASP	3.5
1	A	207	LEU	3.5
1	A	441	PHE	3.5
1	A	434	VAL	3.5
3	D	72	SER	3.4
1	A	9	THR	3.4
1	A	287	GLN	3.4
1	B	183	SER	3.3
1	B	116	GLY	3.3
1	A	292	VAL	3.3
2	C	114	LYS	3.3
2	C	4	ILE	3.3
1	A	439	TYR	3.3
2	E	56	TYR	3.2
1	A	210	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	70	TRP	3.2
1	B	106	ILE	3.2
1	B	117	CYS	3.2
1	A	195	LEU	3.2
1	B	192	PRO	3.1
1	B	265	TRP	3.1
1	B	230	GLU	3.1
1	A	198	THR	3.1
2	C	33	HIS	3.1
2	E	4	ILE	3.1
1	B	324	ASN	3.1
1	B	10	GLY	3.1
1	B	296	TYR	3.0
1	A	418	HIS	3.0
1	A	257	LYS	3.0
1	B	315	TYR	3.0
2	E	58	VAL	2.9
2	C	3	ASP	2.9
2	C	49	GLN	2.9
1	B	33	TYR	2.9
1	B	260	GLY	2.9
3	F	108	ASP	2.8
1	B	158	ARG	2.8
1	A	284	MET	2.8
2	E	72	SER	2.8
1	B	191	TRP	2.7
3	D	104	TYR	2.7
2	E	79	THR	2.7
1	A	166	GLN	2.7
1	B	11	LYS	2.7
1	B	373	TYR	2.7
1	B	93	ASN	2.7
1	A	35	VAL	2.7
1	A	298	TYR	2.7
1	B	240	LYS	2.6
1	A	157	LEU	2.6
1	A	337	LEU	2.6
1	B	391	SER	2.6
1	B	193	ILE	2.6
1	B	301	GLN	2.6
3	D	12	LEU	2.6
2	C	26	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
3	D	27	GLY	2.5
2	E	14	PRO	2.5
1	B	187	SER	2.5
3	D	80	LEU	2.5
1	A	8	LYS	2.5
3	F	105	ASP	2.5
1	B	433	GLN	2.5
3	F	112	GLN	2.5
1	A	37	ALA	2.5
1	A	302	ILE	2.4
1	A	355	CYS	2.4
1	A	356	ILE	2.4
1	B	7	GLU	2.4
3	D	44	LYS	2.4
1	B	34	ASN	2.4
1	A	197	LEU	2.4
1	B	252	GLU	2.4
1	B	400	GLU	2.4
2	E	32	VAL	2.4
1	B	195	LEU	2.4
1	A	117	CYS	2.4
2	C	28	SER	2.3
3	D	89	SER	2.3
2	E	115	THR	2.3
2	E	90	LEU	2.3
3	D	11	GLY	2.3
1	A	310	SER	2.3
1	B	194	LEU	2.3
1	A	116	GLY	2.3
2	C	40	LEU	2.2
1	A	338	TRP	2.2
1	B	198	THR	2.2
1	B	175	VAL	2.2
3	D	109	TYR	2.2
1	B	94	ASN	2.2
1	B	231	LYS	2.2
1	A	468	VAL	2.2
1	B	42	SER	2.2
1	B	156	ASN	2.2
1	B	269	ARG	2.2
3	D	64	THR	2.2
1	A	155	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	109	THR	2.1
1	A	110	LEU	2.1
2	E	71	GLY	2.1
1	A	196	GLY	2.1
2	C	50	SER	2.1
1	B	261	PHE	2.1
1	B	463	LYS	2.1
1	A	464	GLY	2.1
1	B	430	PRO	2.1
3	D	90	GLU	2.1
2	E	113	ILE	2.1
3	D	1	LEU	2.1
1	A	33	TYR	2.1
1	B	355	CYS	2.1
1	B	234	GLN	2.1
3	D	66	LYS	2.0
1	A	320	THR	2.0
1	B	292	VAL	2.0
1	A	393	ILE	2.0
3	D	71	ILE	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.