Full wwPDB X-ray Structure Validation Report (i)

Oct 30, 2023 – 07:14 PM JST

PDB ID	:	4YBQ
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 (i) 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 (1)) were used in the production of this report:

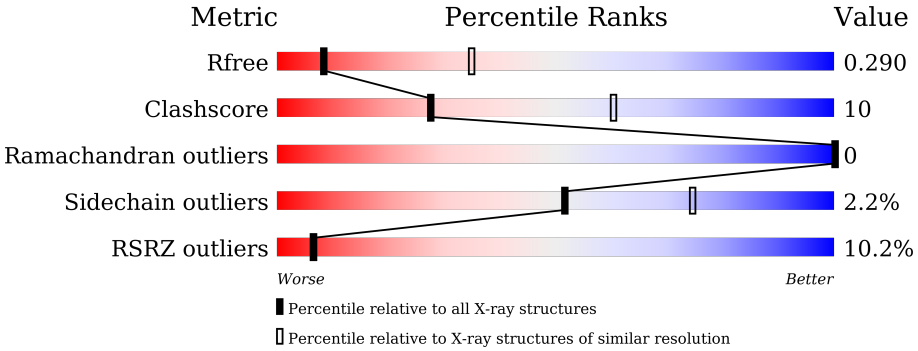
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

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 <=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	9%, 62%, 26%, •, 11%
1	B	508	9%, 65%, 25%, •, 9%
2	C	122	3%, 83%, 11%, 6%
2	E	122	7%, 78%, 16%, 6%
3	D	136	14%, 74%, 15%, 12%
3	F	136	12%, 68%, 19%, •, 12%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	452	3486	2313	553	601	19	0	0	0
1	B	462	3567	2361	567	620	19	0	0	0

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
			Total	C	N	O	S			
2	C	115	885	562	147	174	2	0	0	0
2	E	115	885	562	147	174	2	0	0	0

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

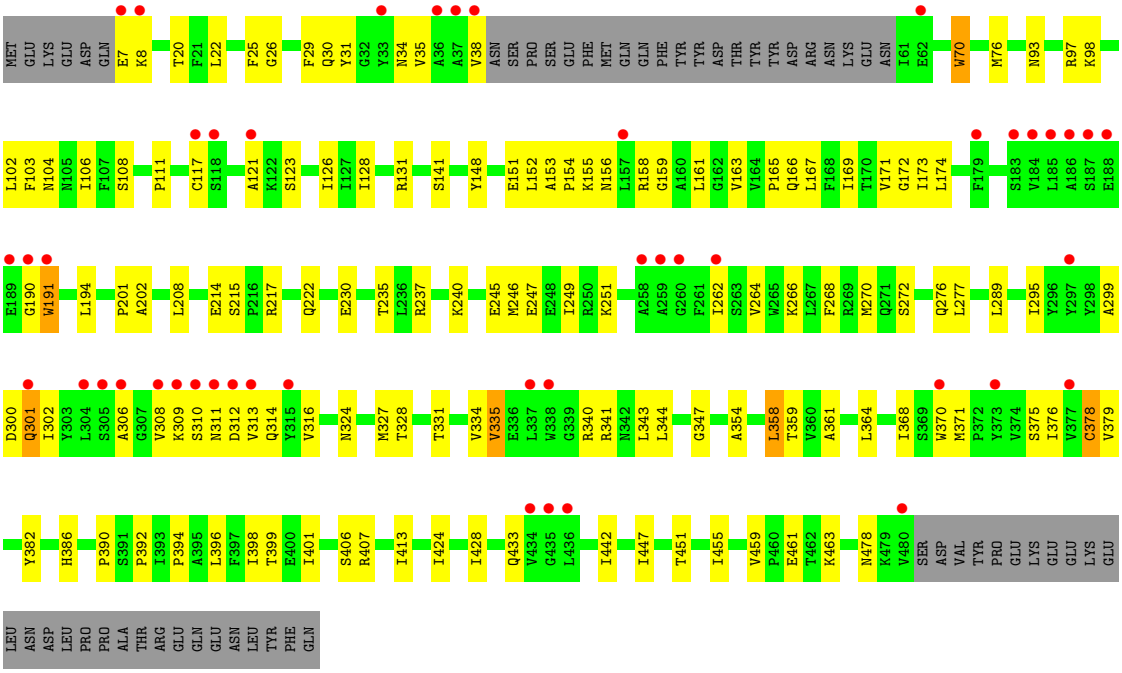
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	120	921	577	160	180	4	0	0	0
			Total	C	N	O	S			
3	F	119	913	571	159	179	4	0	0	0

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.

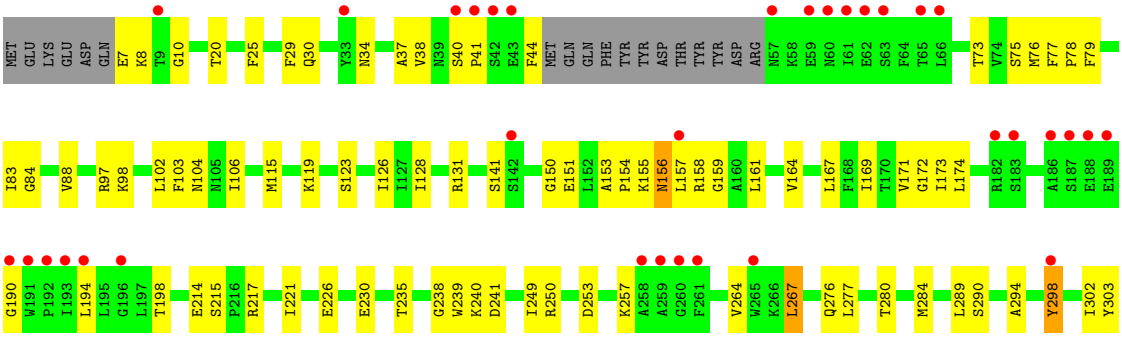
• Molecule 1: Solute carrier family 2, facilitated glucose transporter member 5

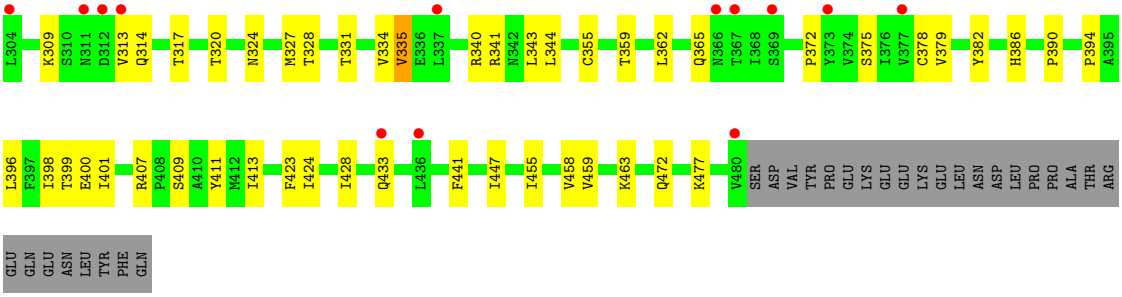
Chain A:



• Molecule 1: Solute carrier family 2, facilitated glucose transporter member 5

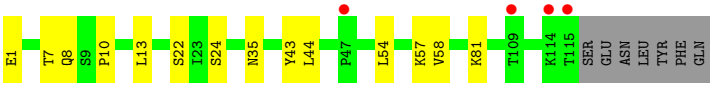
Chain B:





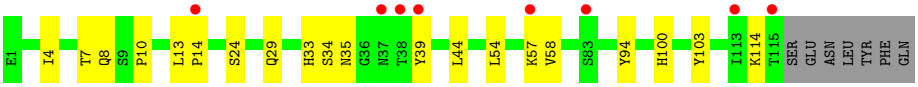
- Molecule 2: antibody Fv fragment light chain

Chain C:



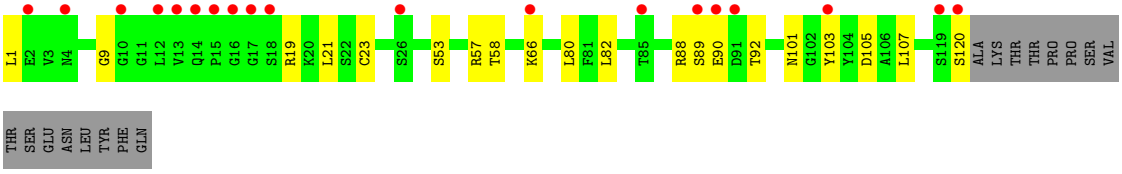
- Molecule 2: antibody Fv fragment light chain

Chain E:



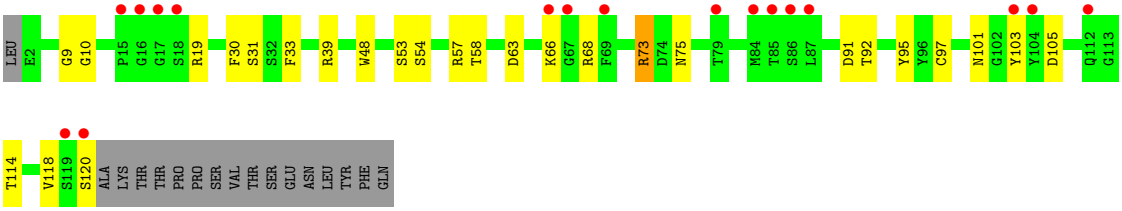
- Molecule 3: antibody Fv fragment heavy chain

Chain D:



- Molecule 3: antibody Fv fragment heavy chain

Chain F:



4 Data and refinement statistics (i)

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 38.08 – 3.24	Depositor EDS
% Data completeness (in resolution range)	99.8 (36.49-3.27) 90.2 (38.08-3.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.99 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.242 , 0.288 0.245 , 0.290	Depositor DCC
R_{free} test set	1877 reflections (4.94%)	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 , 78.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.27	0/3564	0.48	0/4845
1	B	0.27	0/3647	0.47	0/4957
2	C	0.27	0/905	0.50	0/1226
2	E	0.29	0/905	0.53	0/1226
3	D	0.24	0/942	0.52	0/1275
3	F	0.26	0/934	0.56	0/1264
All	All	0.27	0/10897	0.49	0/14793

There are no bond length outliers.

There are no bond angle outliers.

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	91	0
1	B	3567	0	3715	88	0
2	C	885	0	871	10	0
2	E	885	0	871	12	0
3	D	921	0	880	14	0
3	F	913	0	866	20	0
All	All	10657	0	10849	216	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 10.

All (216) 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: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
1:B:7:GLU:OE1	1:B:155:LYS:NZ	2.22	0.66
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
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
1:A:324:ASN:O	1:A:328:THR:OG1	2.16	0.56
1:A:230:GLU:OE1	3:F:57:ARG:NH1	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:311:ASN:OD1	1:A:312:ASP:N	2.40	0.54
1:B:399:THR:OG1	1:B:411:TYR:OH	2.22	0.54
1:A:334:VAL:HG12	1:A:343:LEU:HD11	1.89	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: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: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
1:B:324:ASN:O	1:B:328:THR:OG1	2.20	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:240:LYS:HG3	3:F:105:ASP:CG	2.33	0.49
1:A:266:LYS:O	1:A:270:MET:HG3	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:354:ALA:O	1:A:358:LEU:HB2	2.13	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
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:238:GLY:C	2:C:35:ASN:HD21	2.18	0.45
1:B:267:LEU:HD12	1:B:409:SER:HB2	1.98	0.45
3:F:39:ARG:HD3	3:F:95:TYR:CZ	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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
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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:290:SER:O	1:B:382:TYR:OH	2.39	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 (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	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 (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	378/433 (87%)	367 (97%)	11 (3%)	42	68
1	B	388/433 (90%)	379 (98%)	9 (2%)	50	73
2	C	101/108 (94%)	101 (100%)	0	100	100
2	E	101/108 (94%)	100 (99%)	1 (1%)	76	85
3	D	98/113 (87%)	96 (98%)	2 (2%)	55	76
3	F	97/113 (86%)	94 (97%)	3 (3%)	40	67
All	All	1163/1308 (89%)	1137 (98%)	26 (2%)	52	74

All (26) 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	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	378	CYS
1	B	433	GLN
1	B	472	GLN
3	D	1	LEU
3	D	120	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	29	GLN
3	F	73	ARG
3	F	97	CYS
3	F	120	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	E	33	HIS

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 monosaccharides 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	452/508 (88%)	0.40	46 (10%)	6	6	77, 135, 291, 452	0
1	B	462/508 (90%)	0.49	47 (10%)	6	6	78, 137, 297, 455	0
2	C	115/122 (94%)	0.20	4 (3%)	44	42	91, 127, 188, 232	0
2	E	115/122 (94%)	0.41	8 (6%)	16	16	100, 135, 193, 233	0
3	D	120/136 (88%)	0.64	19 (15%)	2	2	94, 156, 261, 285	0
3	F	119/136 (87%)	0.61	17 (14%)	2	2	94, 159, 264, 286	0
All	All	1383/1532 (90%)	0.45	141 (10%)	6	6	77, 139, 281, 455	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	188	GLU	15.6
1	B	190	GLY	14.0
1	B	259	ALA	13.7
1	B	258	ALA	12.8
1	B	260	GLY	11.4
1	B	480	VAL	10.8
1	A	7	GLU	9.7
1	A	435	GLY	8.4
1	B	192	PRO	8.2
1	B	373	TYR	7.6
1	A	480	VAL	7.3
1	A	187	SER	7.0
1	A	189	GLU	6.8
3	D	119	SER	6.8
1	B	42	SER	6.7
1	B	191	TRP	6.4
1	A	304	LEU	6.3
1	B	312	ASP	6.1
1	A	117	CYS	6.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	118	SER	6.1
1	A	260	GLY	6.0
1	A	259	ALA	5.5
1	B	261	PHE	5.4
1	B	311	ASN	5.1
1	B	41	PRO	5.1
1	B	183	SER	5.0
1	A	38	VAL	4.9
1	B	298	TYR	4.7
3	F	69	PHE	4.7
1	B	193	ILE	4.6
3	F	120	SER	4.6
2	C	114	LYS	4.6
1	A	258	ALA	4.5
3	F	18	SER	4.5
1	A	312	ASP	4.5
2	C	115	THR	4.5
1	B	187	SER	4.4
3	F	119	SER	4.4
1	A	310	SER	4.4
1	A	434	VAL	4.3
2	E	38	THR	4.3
1	B	9	THR	4.3
3	D	89	SER	4.3
1	A	37	ALA	4.2
1	A	305	SER	4.2
3	D	14	GLN	4.1
1	A	370	TRP	4.0
1	B	182	ARG	3.9
1	A	185	LEU	3.9
1	A	121	ALA	3.9
3	D	90	GLU	3.9
1	B	196	GLY	3.9
3	D	12	LEU	3.8
2	E	37	ASN	3.8
3	F	85	THR	3.8
1	B	66	LEU	3.8
1	B	188	GLU	3.7
1	A	33	TYR	3.7
1	A	436	LEU	3.6
1	B	40	SER	3.6
1	B	63	SER	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	D	10	GLY	3.6
3	F	79	THR	3.6
1	A	313	VAL	3.5
1	B	369	SER	3.5
3	D	103	TYR	3.5
1	B	366	ASN	3.4
3	F	67	GLY	3.4
2	E	115	THR	3.4
3	F	103	TYR	3.3
3	F	66	LYS	3.3
3	D	2	GLU	3.3
2	E	57	LYS	3.2
1	B	62	GLU	3.2
1	A	315	TYR	3.1
1	A	62	GLU	3.1
1	A	311	ASN	3.1
3	D	120	SER	3.1
3	F	16	GLY	3.1
3	F	15	PRO	3.1
1	B	57	ASN	3.0
1	B	194	LEU	3.0
1	A	191	TRP	3.0
2	E	113	ILE	3.0
1	B	436	LEU	3.0
1	B	367	THR	3.0
3	D	13	VAL	2.9
3	F	17	GLY	2.9
3	F	104	TYR	2.8
1	A	373	TYR	2.8
1	A	179	PHE	2.8
2	E	39	TYR	2.8
1	B	433	GLN	2.7
2	C	109	THR	2.7
3	F	84	MET	2.7
1	A	184	VAL	2.7
1	A	190	GLY	2.6
1	A	297	TYR	2.6
1	A	186	ALA	2.6
3	D	16	GLY	2.6
3	D	26	SER	2.6
1	B	186	ALA	2.5
3	D	4	ASN	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	157	LEU	2.5
3	F	87	LEU	2.5
1	A	309	LYS	2.5
1	B	61	ILE	2.5
1	A	36	ALA	2.5
1	A	183	SER	2.5
1	A	262	ILE	2.5
1	B	337	LEU	2.4
1	A	306	ALA	2.4
1	B	33	TYR	2.4
1	B	65	THR	2.4
1	B	313	VAL	2.4
1	B	157	LEU	2.4
3	D	18	SER	2.4
3	F	86	SER	2.4
3	D	15	PRO	2.4
3	D	66	LYS	2.3
1	B	265	TRP	2.3
1	A	338	TRP	2.3
1	B	59	GLU	2.3
1	B	60	ASN	2.3
1	B	142	SER	2.2
1	A	301	GLN	2.2
1	B	377	VAL	2.2
3	D	91	ASP	2.1
2	E	14	PRO	2.1
1	B	189	GLU	2.1
1	A	8	LYS	2.1
2	C	47	PRO	2.1
1	B	304	LEU	2.1
3	D	17	GLY	2.1
3	F	112	GLN	2.1
2	E	83	SER	2.1
1	A	308	VAL	2.0
1	A	377	VAL	2.0
3	D	85	THR	2.0
1	A	337	LEU	2.0
1	B	43	GLU	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 monosaccharides 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.