



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 10, 2021 – 10:03 AM EST

PDB ID : 6WJL
Title : Crystal structure of Glypican-2 core protein in complex with D3 Fab
Authors : Raman, S.; Maris, J.M.; Bosse, K.R.; Julien, J.P.
Deposited on : 2020-04-14
Resolution : 3.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
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)	:	2.23.2

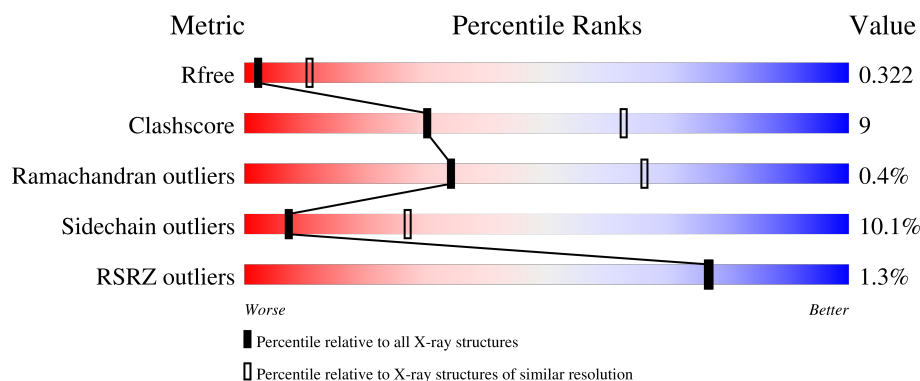
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	E	482	<div> <div>2%</div> <div>60% 20% 5% 16%</div> </div>
1	G	482	<div> <div>%</div> <div>59% 22% 6% 13%</div> </div>
2	F	220	<div> <div>75% 23% ..</div> </div>
2	H	220	<div> <div>78% 20% ..</div> </div>
3	I	121	<div> <div>6%</div> <div>81% 13% 6%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	K	121	<div><div></div><div>2%</div><div>72%</div><div>20%</div><div>5%</div></div>
4	J	214	<div><div></div><div>86%</div><div>14%</div></div>
4	L	214	<div><div></div><div>82%</div><div>16%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14241 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 Glypican-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	419	Total	C	N	O	S	0	0	0
			3209	2021	576	591	21			
1	E	406	Total	C	N	O	S	0	0	0
			3111	1958	559	573	21			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	21	GLU	-	expression tag	UNP Q8N158
G	22	THR	-	expression tag	UNP Q8N158
G	55	THR	SER	engineered mutation	UNP Q8N158
G	92	THR	SER	engineered mutation	UNP Q8N158
G	155	THR	SER	engineered mutation	UNP Q8N158
G	494	GLY	-	expression tag	UNP Q8N158
G	495	THR	-	expression tag	UNP Q8N158
G	496	LYS	-	expression tag	UNP Q8N158
G	497	HIS	-	expression tag	UNP Q8N158
G	498	HIS	-	expression tag	UNP Q8N158
G	499	HIS	-	expression tag	UNP Q8N158
G	500	HIS	-	expression tag	UNP Q8N158
G	501	HIS	-	expression tag	UNP Q8N158
G	502	HIS	-	expression tag	UNP Q8N158
E	21	GLU	-	expression tag	UNP Q8N158
E	22	THR	-	expression tag	UNP Q8N158
E	55	THR	SER	engineered mutation	UNP Q8N158
E	92	THR	SER	engineered mutation	UNP Q8N158
E	155	THR	SER	engineered mutation	UNP Q8N158
E	494	GLY	-	expression tag	UNP Q8N158
E	495	THR	-	expression tag	UNP Q8N158
E	496	LYS	-	expression tag	UNP Q8N158
E	497	HIS	-	expression tag	UNP Q8N158
E	498	HIS	-	expression tag	UNP Q8N158
E	499	HIS	-	expression tag	UNP Q8N158

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	500	HIS	-	expression tag	UNP Q8N158
E	501	HIS	-	expression tag	UNP Q8N158
E	502	HIS	-	expression tag	UNP Q8N158

- Molecule 2 is a protein called D3 Fab Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1639	1039	268	326	6			
2	F	218	Total	C	N	O	S	0	0	0
			1639	1039	268	326	6			

- Molecule 3 is a protein called VHH domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	115	Total	C	N	O	S	0	0	0
			670	407	126	135	2			
3	I	114	Total	C	N	O	S	0	0	0
			687	420	129	136	2			

- Molecule 4 is a protein called D3 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	213	Total	C	N	O	S	0	0	0
			1643	1032	275	331	5			
4	J	213	Total	C	N	O	S	0	0	0
			1643	1032	275	331	5			



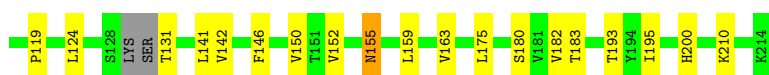
- Molecule 2: D3 Fab Heavy chain

Chain H: 78% 20% ..



- Molecule 2: D3 Fab Heavy chain

Chain F: 75% 23% ..



- Molecule 3: VHH domain

Chain K: 2% 72% 20% 5%



- Molecule 3: VHH domain

Chain I: 6% 81% 13% 6%



- Molecule 4: D3 Fab Light Chain

Chain L: 82% 16%

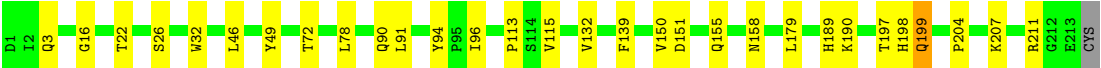


- Molecule 4: D3 Fab Light Chain

Chain J:

86%

14%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.94Å 225.65Å 107.25Å 90.00° 104.75° 90.00°	Depositor
Resolution (Å)	29.48 – 3.30 29.48 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.48-3.30) 95.2 (29.48-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.31Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.278 , 0.317 0.284 , 0.322	Depositor DCC
R_{free} test set	1833 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	72.4	Xtriage
Anisotropy	0.359	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 20.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.390 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	14241	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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	E	0.29	0/3169	0.48	0/4287
1	G	0.34	1/3271 (0.0%)	0.54	0/4431
2	F	0.25	0/1679	0.47	0/2286
2	H	0.25	0/1679	0.47	0/2286
3	I	0.28	0/332	0.46	0/413
3	K	0.42	0/304	0.57	0/376
4	J	0.25	0/1679	0.45	0/2281
4	L	0.26	0/1679	0.46	0/2281
All	All	0.29	1/13792 (0.0%)	0.49	0/18641

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	175	PHE	C-N	8.79	1.50	1.34

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	E	3111	0	3077	55	0
1	G	3209	0	3171	81	0
2	F	1639	0	1591	29	0
2	H	1639	0	1591	28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	687	0	400	16	0
3	K	670	0	366	22	0
4	J	1643	0	1604	22	0
4	L	1643	0	1604	23	0
All	All	14241	0	13404	257	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 9.

All (257) 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:I:12:VAL:HG21	3:I:16:UNK:CB	1.56	1.35
3:I:12:VAL:CG2	3:I:16:UNK:CB	2.11	1.29
3:I:106:UNK:CB	4:J:198:HIS:C	2.08	1.20
1:G:465:VAL:HG13	1:G:466:PRO:HD3	1.32	1.11
3:K:106:UNK:CB	4:L:198:HIS:C	2.29	0.99
3:I:12:VAL:HG22	3:I:16:UNK:CB	1.94	0.97
3:K:106:UNK:CB	4:L:199:GLN:N	2.30	0.94
3:I:106:UNK:CB	4:J:198:HIS:CA	2.45	0.93
3:K:16:UNK:O	3:K:86:LEU:HG	1.72	0.88
1:E:286:SER:OG	1:E:462:GLY:O	1.92	0.86
3:I:106:UNK:CB	4:J:199:GLN:N	2.41	0.82
1:G:286:SER:OG	1:G:464:ASP:OD1	1.99	0.81
3:K:17:SER:HB3	3:K:84:UNK:HA	1.63	0.79
4:L:32:TRP:HB3	4:L:91:LEU:HB2	1.67	0.76
1:G:286:SER:CB	1:G:464:ASP:OD1	2.34	0.75
3:K:86:LEU:HD23	3:K:86:LEU:N	2.02	0.74
1:E:397:ARG:NH2	2:F:95:GLU:OE2	2.18	0.74
1:G:308:GLN:HB2	1:G:391:VAL:HG21	1.67	0.74
1:G:237:VAL:HG22	1:G:474:LEU:HD13	1.68	0.74
1:G:175:PHE:HB3	1:G:176:PRO:HD3	1.71	0.72
2:H:87:THR:HG23	2:H:110:ALA:HA	1.72	0.72
1:G:42:ARG:NE	1:G:80:GLU:OE2	2.21	0.72
1:G:339:SER:HA	1:G:342:VAL:HG22	1.72	0.70
1:G:397:ARG:NH1	2:H:95:GLU:OE2	2.23	0.70
4:J:3:GLN:HG2	4:J:26:SER:HB2	1.73	0.69
1:G:266:VAL:HG23	1:G:268:SER:H	1.58	0.68
2:F:22:CYS:HB3	2:F:78:LEU:HB3	1.76	0.67
3:K:106:UNK:CB	4:L:198:HIS:CA	2.73	0.67
1:G:272:CYS:N	1:G:429:CYS:SG	2.58	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:ARG:HE	1:E:245:PRO:HA	1.59	0.66
1:G:54:ILE:HG23	1:G:55:THR:H	1.61	0.65
1:E:39:LEU:HD11	1:E:262:LEU:HD11	1.79	0.65
4:J:115:VAL:HG13	4:J:207:LYS:HE2	1.79	0.65
3:I:106:UNK:CB	4:J:198:HIS:HA	2.27	0.65
1:E:330:TYR:O	1:E:334:ASN:HB2	1.97	0.64
1:E:330:TYR:CZ	1:E:334:ASN:ND2	2.64	0.64
2:F:93:ALA:HB1	2:F:100(B):PHE:HB3	1.80	0.64
1:G:82:GLU:OE2	1:G:251:SER:OG	2.11	0.63
1:G:154:GLU:OE1	1:G:229:GLN:NE2	2.32	0.63
1:G:465:VAL:CG1	1:G:466:PRO:HD3	2.19	0.62
1:E:54:ILE:HG23	1:E:55:THR:HG23	1.81	0.62
1:E:47:ASN:OD1	1:E:47:ASN:N	2.21	0.61
4:J:32:TRP:HB3	4:J:91:LEU:HB2	1.82	0.61
2:F:193:THR:HB	2:F:210:LYS:HE2	1.82	0.61
1:E:250:CYS:HA	1:E:456:LEU:HD11	1.82	0.61
4:L:197:THR:HG22	4:L:204:PRO:HB3	1.81	0.60
3:K:17:SER:CB	3:K:84:UNK:HA	2.31	0.60
1:E:45:SER:HB2	1:E:48:LEU:HD23	1.83	0.60
1:E:248:GLU:O	1:E:252:GLN:NE2	2.35	0.60
1:E:342:VAL:HG12	1:E:342:VAL:O	2.02	0.59
1:G:147:ARG:NH1	1:G:165:ASP:OD2	2.35	0.59
1:E:343:PHE:HD1	1:E:343:PHE:O	1.85	0.59
1:E:279:VAL:HA	1:E:456:LEU:HD23	1.84	0.59
3:I:54:UNK:O	3:I:55:UNK:CB	2.51	0.59
1:E:165:ASP:HB3	1:E:169:GLN:HE22	1.68	0.59
1:E:281:ARG:NH1	1:E:443:VAL:O	2.36	0.58
1:G:34:GLU:OE2	1:G:266:VAL:HG12	2.03	0.58
2:H:22:CYS:HB3	2:H:78:LEU:HB3	1.85	0.58
1:G:115:LEU:HD13	1:G:149:ARG:HG2	1.87	0.57
1:E:299:GLY:HA3	1:E:478:THR:HG23	1.86	0.57
4:L:189:HIS:O	4:L:211:ARG:NH1	2.38	0.56
1:G:449:GLU:OE1	1:G:449:GLU:N	2.38	0.56
1:G:452:ASN:OD1	1:G:452:ASN:N	2.38	0.56
1:E:452:ASN:OD1	1:E:452:ASN:N	2.39	0.56
2:H:52:SER:O	2:H:71:ARG:NH1	2.39	0.56
1:G:453:ASN:N	1:G:453:ASN:OD1	2.38	0.56
3:I:39:GLN:HB2	3:I:45:ARG:HG3	1.87	0.56
1:E:46:LEU:HD23	1:E:46:LEU:H	1.71	0.55
3:K:73:ASP:OD2	3:K:76:UNK:N	2.40	0.55
1:E:257:LEU:HD11	1:E:276:CYS:HA	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:52:SER:O	2:F:71:ARG:NH1	2.40	0.55
1:G:244:VAL:HG22	1:G:245:PRO:HD2	1.88	0.54
2:F:59:TYR:O	4:J:94:TYR:OH	2.25	0.54
4:J:151:ASP:OD2	4:J:189:HIS:HB3	2.07	0.54
3:K:33:UNK:CB	3:K:52:UNK:HA	2.37	0.54
1:G:439:LEU:N	1:G:440:PRO:HD3	2.22	0.54
1:E:233:THR:O	1:E:237:VAL:HG23	2.08	0.54
2:H:51:ILE:HG23	2:H:71:ARG:HH11	1.72	0.54
2:F:142:VAL:HG11	2:F:150:VAL:HG21	1.90	0.54
1:G:316:THR:HA	1:G:319:SER:HB3	1.88	0.54
3:I:82:GLN:NE2	3:I:83:UNK:O	2.40	0.54
1:G:287:ARG:NH1	1:G:464:ASP:OD1	2.41	0.53
4:L:155:GLN:OE1	4:L:158:ASN:ND2	2.41	0.53
1:E:200:ASP:OD1	1:E:201:GLY:N	2.40	0.53
4:L:89:GLN:HG2	4:L:90:GLN:H	1.74	0.53
1:G:227:PHE:HB2	1:G:303:LEU:HD13	1.91	0.53
2:H:35:SER:HA	2:H:50:TYR:HA	1.91	0.53
4:L:155:GLN:HB3	4:L:158:ASN:HD21	1.72	0.52
1:G:431:THR:OG1	1:G:434:GLY:O	2.22	0.52
1:G:172:GLU:HB3	1:G:195:LEU:HD13	1.90	0.52
1:E:229:GLN:OE1	1:E:480:ARG:NH2	2.42	0.52
1:G:261:PRO:HG3	1:G:430:TRP:CD2	2.44	0.52
1:E:447:PRO:HA	1:E:450:GLN:HB3	1.92	0.51
4:J:113:PRO:HA	4:J:139:PHE:HB3	1.92	0.51
3:I:106:UNK:CB	4:J:198:HIS:O	2.55	0.51
4:J:22:THR:HG22	4:J:72:THR:HG22	1.92	0.51
4:L:37:GLN:HB2	4:L:47:LEU:HD11	1.91	0.51
2:F:5:VAL:HG13	2:F:23:ALA:HB3	1.92	0.51
1:G:253:ALA:HB1	1:G:256:ARG:HE	1.74	0.51
2:H:147:PRO:HD2	2:H:202:PRO:HG2	1.93	0.51
4:J:132:VAL:HB	4:J:179:LEU:HB3	1.91	0.51
1:E:478:THR:O	1:E:482:LYS:N	2.28	0.51
1:G:335:SER:HA	1:G:338:VAL:HG12	1.93	0.51
1:G:103:ARG:HH21	1:G:106:LYS:HD2	1.76	0.51
2:H:163:VAL:HG22	2:H:182:VAL:HG22	1.93	0.50
1:G:160:ASP:OD1	1:G:160:ASP:N	2.43	0.50
1:G:446:SER:HB3	1:G:447:PRO:HD2	1.94	0.50
2:F:159:LEU:HD21	2:F:182:VAL:HG11	1.94	0.50
3:K:36:TRP:CG	3:K:81:LEU:HD12	2.45	0.50
1:E:145:PHE:HA	1:E:148:LEU:HB2	1.93	0.50
4:L:24:ARG:NE	4:L:70:GLU:OE2	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:10:GLY:O	3:K:117:VAL:HG13	2.13	0.49
1:G:417:ARG:HD3	1:G:417:ARG:N	2.26	0.49
2:F:100(A):VAL:HG11	4:J:49:TYR:HB2	1.95	0.49
4:J:197:THR:HG22	4:J:204:PRO:HB3	1.95	0.48
1:E:463:PRO:HB2	1:E:468:ARG:HH21	1.77	0.48
2:H:93:ALA:HB1	2:H:100(B):PHE:HB3	1.95	0.48
1:G:437:ARG:HE	1:G:437:ARG:HA	1.77	0.48
4:L:16:GLY:H	4:L:78:LEU:HB3	1.79	0.48
1:G:49:ILE:H	1:G:50:PRO:HD3	1.78	0.48
1:G:392:TRP:HA	1:G:395:ARG:HB2	1.95	0.48
2:F:163:VAL:HG22	2:F:182:VAL:HG22	1.96	0.47
1:G:477:ALA:O	1:G:481:MET:N	2.44	0.47
2:H:34:MET:HB3	2:H:78:LEU:HD22	1.96	0.47
1:E:271:PRO:HA	1:E:429:CYS:HB3	1.96	0.47
2:F:152:VAL:HG11	2:F:180:SER:OG	2.14	0.47
1:E:227:PHE:HB2	1:E:303:LEU:HD13	1.96	0.47
3:I:105:UNK:O	3:I:106:UNK:CB	2.60	0.47
4:J:113:PRO:HD3	4:J:198:HIS:ND1	2.29	0.47
1:G:446:SER:O	1:G:450:GLN:N	2.40	0.47
1:E:244:VAL:HB	1:E:287:ARG:HE	1.79	0.47
1:G:70:SER:HB2	1:G:73:THR:HG23	1.97	0.47
3:K:86:LEU:N	3:K:86:LEU:CD2	2.72	0.47
3:K:33:UNK:CB	3:K:51:UNK:O	2.62	0.47
2:F:98:TYR:O	2:F:100(A):VAL:HG22	2.14	0.47
1:G:61:VAL:HG21	1:G:255:MET:HB3	1.96	0.47
2:H:193:THR:HB	2:H:210:LYS:HE3	1.95	0.47
3:K:18:LEU:HA	3:K:18:LEU:HD23	1.72	0.47
4:L:158:ASN:N	4:L:158:ASN:OD1	2.47	0.47
2:H:51:ILE:HD13	2:H:71:ARG:HB2	1.96	0.47
1:G:250:CYS:HB2	1:G:456:LEU:HD21	1.97	0.47
3:K:88:UNK:HA	3:K:119:VAL:HG21	1.97	0.47
3:K:21:SER:HA	3:K:80:UNK:HA	1.97	0.46
1:E:471:ARG:O	1:E:475:ARG:NE	2.45	0.46
2:H:189:LEU:HB3	2:H:213:PRO:HG3	1.96	0.46
1:E:431:THR:HG22	1:E:432:GLY:H	1.78	0.46
1:E:464:ASP:HB3	1:E:466:PRO:HD2	1.96	0.46
1:G:195:LEU:HD23	1:G:196:ALA:H	1.81	0.46
2:H:121:VAL:HG12	2:H:209:LYS:HD3	1.98	0.46
3:K:68:PHE:HB3	3:K:81:LEU:HD21	1.98	0.46
3:K:69:THR:HG22	3:K:70:UNK:H	1.79	0.46
2:F:33:TYR:HB2	2:F:95:GLU:HB3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:257:LEU:HD13	1:G:279:VAL:HG21	1.97	0.46
1:G:442:VAL:O	1:G:442:VAL:HG13	2.16	0.46
2:F:101:ASP:HB3	4:J:46:LEU:HD23	1.96	0.46
4:J:16:GLY:N	4:J:78:LEU:O	2.46	0.46
4:L:33:LEU:HD22	4:L:71:PHE:CG	2.50	0.46
1:E:203:LEU:HD12	1:E:203:LEU:HA	1.82	0.46
4:L:14:PHE:HB2	4:L:17:ASP:OD2	2.16	0.45
1:E:389:ARG:O	1:E:393:GLU:HB2	2.16	0.45
1:E:470:ARG:HA	1:E:474:LEU:HD12	1.98	0.45
1:G:453:ASN:ND2	1:G:458:VAL:H	2.15	0.45
1:G:193:SER:O	1:G:194:ARG:HD2	2.16	0.45
1:G:277:LEU:HB2	1:G:442:VAL:CG2	2.46	0.45
1:G:273:GLN:CD	1:G:273:GLN:H	2.20	0.45
1:G:472:LEU:HA	1:G:475:ARG:HH21	1.82	0.45
2:H:67:PHE:HD1	2:H:80:LEU:HD11	1.82	0.45
1:G:478:THR:HA	1:G:481:MET:HE2	1.98	0.45
2:H:119:PRO:HB2	2:H:142:VAL:HG13	1.98	0.45
2:F:66:ARG:HB2	2:F:82(A):ASN:O	2.17	0.45
1:G:49:ILE:N	1:G:50:PRO:CD	2.80	0.45
1:E:93:GLY:HA3	1:E:404:PHE:CZ	2.52	0.45
3:I:4:LEU:HD21	3:I:96:CYS:SG	2.57	0.45
3:I:106:UNK:CB	4:J:198:HIS:N	2.80	0.45
1:E:343:PHE:O	1:E:343:PHE:CD1	2.69	0.44
1:E:456:LEU:HD13	1:E:456:LEU:HA	1.57	0.44
1:G:209:SER:N	1:G:210:PRO:HD2	2.32	0.44
3:K:18:LEU:O	3:K:83:UNK:N	2.50	0.44
1:G:233:THR:O	1:G:237:VAL:HG23	2.17	0.44
2:H:39:GLN:HB2	2:H:45:LEU:HD23	2.00	0.44
2:H:124:LEU:HD11	2:H:141:LEU:HB2	1.99	0.44
2:F:89:VAL:HA	2:F:108:LEU:HA	1.98	0.44
3:K:106:UNK:CB	4:L:198:HIS:HA	2.47	0.44
1:E:462:GLY:N	1:E:463:PRO:CD	2.81	0.44
3:I:4:LEU:C	3:I:4:LEU:HD23	2.37	0.44
2:H:60:ALA:HB3	2:H:63:VAL:HG22	1.98	0.44
1:E:101:ALA:HB2	1:E:235:ARG:HE	1.82	0.44
1:E:165:ASP:HB3	1:E:169:GLN:NE2	2.33	0.44
2:H:124:LEU:HB3	4:L:118:PHE:CD2	2.52	0.44
1:G:344:GLN:H	1:G:344:GLN:HG2	1.45	0.44
2:F:39:GLN:HB2	2:F:45:LEU:HD23	2.00	0.44
1:E:213:LEU:HD11	1:E:320:ILE:HG12	1.99	0.43
1:G:73:THR:O	1:G:77:LEU:N	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:49:ILE:H	1:G:50:PRO:CD	2.32	0.43
4:L:94:TYR:CD2	4:L:95:PRO:HD3	2.53	0.43
3:I:18:LEU:HD23	3:I:18:LEU:HA	1.82	0.43
2:H:206:LYS:HE2	2:H:206:LYS:HB3	1.90	0.43
3:K:118:THR:HG22	3:K:119:VAL:H	1.82	0.43
1:G:303:LEU:HG	1:G:481:MET:O	2.19	0.43
1:G:335:SER:HA	1:G:338:VAL:CG1	2.49	0.43
4:L:145:LYS:HB3	4:L:197:THR:OG1	2.19	0.43
1:E:407:ARG:HE	1:E:407:ARG:HB2	1.61	0.43
2:F:96:SER:HB3	2:F:101:ASP:CG	2.39	0.43
4:J:190:LYS:HE2	4:J:190:LYS:HB3	1.85	0.43
1:G:400:ARG:HG2	2:H:31:ASP:HA	2.01	0.43
1:E:303:LEU:HD12	1:E:481:MET:HB3	2.00	0.43
1:G:462:GLY:N	1:G:463:PRO:CD	2.82	0.42
1:G:192:LEU:HD23	1:G:193:SER:H	1.84	0.42
1:G:261:PRO:HG3	1:G:430:TRP:CG	2.54	0.42
1:E:398:LEU:HA	1:E:401:MET:HE3	2.01	0.42
1:E:450:GLN:OE1	1:E:453:ASN:ND2	2.51	0.42
1:E:451:VAL:HG22	1:E:458:VAL:HG11	2.02	0.42
2:F:12:VAL:HG23	2:F:111:VAL:HG12	2.02	0.42
1:G:145:PHE:HA	1:G:148:LEU:HD12	2.01	0.42
3:K:48:VAL:O	3:K:61:UNK:N	2.53	0.42
2:H:67:PHE:CE1	2:H:82:MET:HG2	2.55	0.42
1:E:289:LEU:H	1:E:289:LEU:HG	1.68	0.42
2:H:95:GLU:HG2	2:H:97:GLY:H	1.84	0.42
1:G:77:LEU:HD22	1:G:255:MET:HE1	2.01	0.42
1:E:457:LYS:HD3	1:E:457:LYS:HA	1.65	0.42
1:G:186:PRO:HB3	1:G:191:CYS:SG	2.59	0.42
1:G:209:SER:OG	1:G:326:GLU:OE1	2.38	0.42
1:G:77:LEU:HB3	1:G:255:MET:HE1	2.02	0.42
1:G:229:GLN:HB3	1:G:480:ARG:HH22	1.83	0.42
1:G:337:LYS:N	1:G:337:LYS:CD	2.78	0.42
2:H:124:LEU:HD23	4:L:118:PHE:CD1	2.54	0.42
1:E:49:ILE:H	1:E:49:ILE:HG12	1.50	0.42
2:F:124:LEU:HD21	2:F:141:LEU:HB2	2.01	0.42
2:F:146:PHE:HB2	2:F:175:LEU:HD22	2.02	0.41
1:G:253:ALA:HB1	1:G:256:ARG:NE	2.35	0.41
1:E:261:PRO:HG3	1:E:430:TRP:CD2	2.56	0.41
4:L:50:ALA:O	4:L:52:SER:N	2.49	0.41
1:G:73:THR:O	1:G:77:LEU:HB2	2.20	0.41
2:H:67:PHE:CZ	2:H:82:MET:HG2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:30:SER:OG	4:L:31:SER:N	2.54	0.41
1:E:411:THR:HG23	2:F:28:THR:HG23	2.03	0.41
1:G:286:SER:OG	1:G:464:ASP:CG	2.58	0.41
2:H:86:ASP:O	2:H:90:TYR:OH	2.35	0.41
2:F:36:TRP:CE2	2:F:80:LEU:HB2	2.56	0.41
1:G:256:ARG:O	1:G:430:TRP:NE1	2.53	0.41
1:G:453:ASN:ND2	1:G:456:LEU:O	2.54	0.41
2:H:33:TYR:HB2	2:H:95:GLU:HB3	2.02	0.41
2:F:119:PRO:HB2	2:F:142:VAL:HG13	2.03	0.41
4:J:132:VAL:O	4:J:179:LEU:N	2.42	0.41
4:J:150:VAL:HB	4:J:155:GLN:HE21	1.85	0.41
1:G:281:ARG:O	1:G:285:SER:N	2.54	0.41
2:F:155:ASN:OD1	2:F:155:ASN:N	2.54	0.41
1:G:446:SER:HB2	1:G:449:GLU:OE1	2.22	0.40
1:E:49:ILE:HG23	1:E:73:THR:HG21	2.02	0.40
1:E:169:GLN:O	1:E:172:GLU:HG2	2.21	0.40
2:F:150:VAL:HG12	2:F:200:HIS:HD2	1.86	0.40
1:G:229:GLN:OE1	1:G:480:ARG:NH1	2.45	0.40
1:G:277:LEU:HB2	1:G:442:VAL:HG21	2.03	0.40
1:G:331:LEU:O	1:G:335:SER:N	2.53	0.40
2:F:2:VAL:HG13	2:F:27:PHE:CD2	2.57	0.40
2:F:39:GLN:O	2:F:89:VAL:HG12	2.22	0.40
4:L:52:SER:HA	4:L:64:GLY:O	2.21	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	E	392/482 (81%)	355 (91%)	34 (9%)	3 (1%)	19 51
1	G	409/482 (85%)	367 (90%)	39 (10%)	3 (1%)	22 54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	214/220 (97%)	195 (91%)	19 (9%)	0	100	100
2	H	214/220 (97%)	203 (95%)	10 (5%)	1 (0%)	29	61
3	I	44/121 (36%)	37 (84%)	7 (16%)	0	100	100
3	K	44/121 (36%)	39 (89%)	5 (11%)	0	100	100
4	J	211/214 (99%)	203 (96%)	8 (4%)	0	100	100
4	L	211/214 (99%)	202 (96%)	9 (4%)	0	100	100
All	All	1739/2074 (84%)	1601 (92%)	131 (8%)	7 (0%)	34	66

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	442	VAL
1	E	140	ILE
1	G	247	SER
1	E	344	GLN
1	G	51	PRO
1	E	346	CYS
2	H	147	PRO

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	E	332/400 (83%)	279 (84%)	53 (16%)	2	11
1	G	341/400 (85%)	288 (84%)	53 (16%)	2	12
2	F	183/185 (99%)	171 (93%)	12 (7%)	16	46
2	H	183/185 (99%)	174 (95%)	9 (5%)	25	56
3	I	37/39 (95%)	34 (92%)	3 (8%)	11	36
3	K	32/39 (82%)	26 (81%)	6 (19%)	1	6
4	J	187/188 (100%)	182 (97%)	5 (3%)	44	71
4	L	187/188 (100%)	178 (95%)	9 (5%)	25	56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1482/1624 (91%)	1332 (90%)	150 (10%)	7 27

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	32	CYS
1	G	46	LEU
1	G	48	LEU
1	G	49	ILE
1	G	53	LEU
1	G	55	THR
1	G	77	LEU
1	G	90	GLU
1	G	109	GLU
1	G	133	LEU
1	G	154	GLU
1	G	160	ASP
1	G	163	LEU
1	G	177	LEU
1	G	179	HIS
1	G	182	TYR
1	G	191	CYS
1	G	192	LEU
1	G	194	ARG
1	G	195	LEU
1	G	200	ASP
1	G	204	GLN
1	G	206	PHE
1	G	208	ASP
1	G	244	VAL
1	G	246	VAL
1	G	250	CYS
1	G	254	LEU
1	G	262	LEU
1	G	266	VAL
1	G	269	LEU
1	G	275	PHE
1	G	279	VAL
1	G	303	LEU
1	G	311	PHE
1	G	316	THR
1	G	343	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	344	GLN
1	G	346	CYS
1	G	392	TRP
1	G	394	LEU
1	G	396	GLU
1	G	417	ARG
1	G	437	ARG
1	G	452	ASN
1	G	455	GLU
1	G	456	LEU
1	G	458	VAL
1	G	465	VAL
1	G	467	THR
1	G	475	ARG
1	G	480	ARG
1	G	488	HIS
2	H	50	TYR
2	H	61	ASP
2	H	82(C)	LEU
2	H	108	LEU
2	H	138	LEU
2	H	183	THR
2	H	209	LYS
2	H	212	GLU
2	H	214	LYS
3	K	12	VAL
3	K	13	GLN
3	K	17	SER
3	K	69	THR
3	K	86	LEU
3	K	118	THR
4	L	15	VAL
4	L	29	ILE
4	L	90	GLN
4	L	94	TYR
4	L	123	GLU
4	L	152	ASN
4	L	158	ASN
4	L	190	LYS
4	L	205	VAL
1	E	44	TYR
1	E	47	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	49	ILE
1	E	61	VAL
1	E	68	CYS
1	E	79	ARG
1	E	96	LEU
1	E	114	MET
1	E	125	LEU
1	E	130	TYR
1	E	140	ILE
1	E	154	GLU
1	E	155	THR
1	E	163	LEU
1	E	169	GLN
1	E	174	VAL
1	E	175	PHE
1	E	179	HIS
1	E	199	THR
1	E	246	VAL
1	E	247	SER
1	E	248	GLU
1	E	252	GLN
1	E	263	CYS
1	E	269	LEU
1	E	273	GLN
1	E	278	ASN
1	E	289	LEU
1	E	303	LEU
1	E	316	THR
1	E	334	ASN
1	E	339	SER
1	E	343	PHE
1	E	346	CYS
1	E	380	THR
1	E	393	GLU
1	E	394	LEU
1	E	396	GLU
1	E	413	CYS
1	E	424	LEU
1	E	429	CYS
1	E	431	THR
1	E	435	ARG
1	E	439	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	450	GLN
1	E	452	ASN
1	E	456	LEU
1	E	458	VAL
1	E	467	THR
1	E	474	LEU
1	E	475	ARG
1	E	478	THR
1	E	480	ARG
2	F	5	VAL
2	F	11	VAL
2	F	50	TYR
2	F	56	THR
2	F	82	MET
2	F	82(C)	LEU
2	F	98	TYR
2	F	99	ASP
2	F	131	THR
2	F	155	ASN
2	F	183	THR
2	F	195	ILE
3	I	20	LEU
3	I	69	THR
3	I	73	ASP
4	J	90	GLN
4	J	96	ILE
4	J	158	ASN
4	J	199	GLN
4	J	211	ARG

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

Mol	Chain	Res	Type
3	K	82	GLN

5.3.3 RNA ⓘ

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 ⓘ

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	E	406/482 (84%)	-0.14	8 (1%) 65 64	34, 87, 116, 149	0
1	G	419/482 (86%)	-0.16	6 (1%) 75 75	42, 86, 115, 136	0
2	F	218/220 (99%)	-0.32	0 100 100	33, 64, 97, 120	0
2	H	218/220 (99%)	-0.28	1 (0%) 91 91	32, 63, 87, 106	0
3	I	46/121 (38%)	0.45	7 (15%) 2 2	76, 96, 115, 128	0
3	K	45/121 (37%)	0.15	2 (4%) 34 33	74, 92, 109, 116	0
4	J	213/214 (99%)	-0.30	0 100 100	36, 55, 76, 90	0
4	L	213/214 (99%)	-0.31	0 100 100	32, 56, 76, 94	0
All	All	1778/2074 (85%)	-0.20	24 (1%) 77 77	32, 69, 111, 149	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	96	CYS	3.9
3	K	8	GLY	3.8
1	E	157	GLU	3.4
1	E	155	THR	3.4
1	G	441	PRO	3.3
3	I	7	SER	3.2
2	H	179	SER	3.2
3	I	8	GLY	3.2
1	G	384	GLY	2.6
1	E	193	SER	2.5
1	G	442	VAL	2.5
1	G	190	LEU	2.4
1	E	284	LEU	2.4
3	I	21	SER	2.3
1	G	426	ALA	2.2
3	K	7	SER	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	382	ALA	2.2
1	G	347	GLY	2.2
1	E	179	HIS	2.1
3	I	18	LEU	2.1
1	E	128	HIS	2.1
3	I	119	VAL	2.0
1	E	68	CYS	2.0
3	I	4	LEU	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.