



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 07:54 am BST

PDB ID : 1VYT
Title : beta3 subunit complexed with aid
Authors : Chen, Y.-H.; Li, M.-H.; Zhang, Y.; He, L.-L.; Yamada, Y.; Fitzmaurice, A.;
Yang, S.; Zhang, H.; Tong, L.; Yang, J.
Deposited on : 2004-05-07
Resolution : 2.60 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	:	2.11
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)	:	2.11

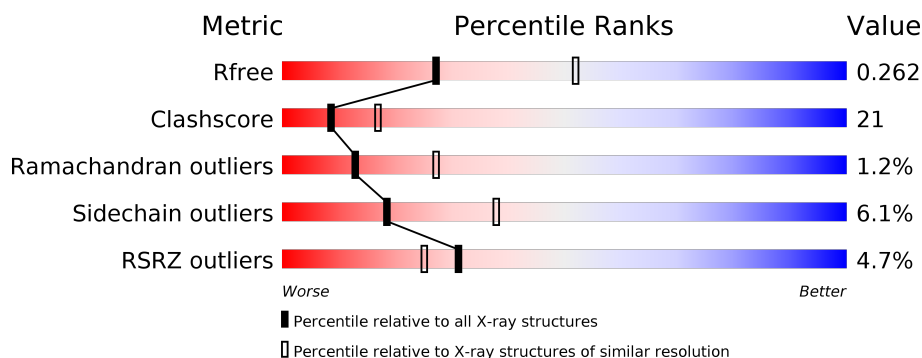
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 on 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	351	<div> <div>4%</div> <div> <div></div> <div>50%</div> <div>26%</div> <div>•</div> <div>22%</div> </div> </div>
1	B	351	<div> <div>3%</div> <div> <div></div> <div>51%</div> <div>28%</div> <div>5%</div> <div>16%</div> </div> </div>
2	E	25	<div> <div></div> <div> <div>64%</div> <div>20%</div> <div>16%</div> </div> </div>
2	F	25	<div> <div>16%</div> <div> <div>12%</div> <div>40%</div> <div>16%</div> <div>32%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4962 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 CALCIUM CHANNEL BETA-3 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	0	0	1
			2184	1386	384	404	10			
1	B	295	Total	C	N	O	S	0	0	1
			2348	1484	420	434	10			

- Molecule 2 is a protein called VOLTAGE-DEPENDENT L-TYPE CALCIUM CHANNEL ALPHA-1C SUBUNIT.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	25	Total	C	N	O	0	0	0
			217	135	36	46			
2	F	17	Total	C	N	O	0	0	1
			136	87	20	29			

- Molecule 3 is water.

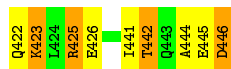
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	45	Total	O	0	0
			45	45		
3	B	26	Total	O	0	0
			26	26		
3	E	6	Total	O	0	0
			6	6		

- Molecule 1: CALCIUM CHANNEL BETA-3 SUBUNIT



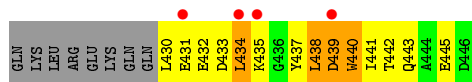
- Molecule 2: VOLTAGE-DEPENDENT L-TYPE CALCIUM CHANNEL ALPHA-1C SUB-UNIT

Chain E: 



- Molecule 2: VOLTAGE-DEPENDENT L-TYPE CALCIUM CHANNEL ALPHA-1C SUB-UNIT

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	252.30 Å 69.00 Å 60.70 Å 90.00° 96.70° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60 29.51 – 2.61	Depositor EDS
% Data completeness (in resolution range)	96.0 (30.00-2.60) 95.9 (29.51-2.61)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.27 (at 2.61 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.231 , 0.272 0.221 , 0.262	Depositor DCC
R_{free} test set	3157 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	45.8	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 46.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4962	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.37% 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	0.44	0/2226	0.65	0/3009
1	B	0.38	0/2393	0.64	2/3234 (0.1%)
2	E	0.43	0/219	0.54	0/291
2	F	0.51	0/138	0.81	0/187
All	All	0.42	0/4976	0.64	2/6721 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295	SER	N-CA-C	5.63	126.21	111.00
1	B	294	VAL	N-CA-C	-5.05	97.37	111.00

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	2184	0	2204	80	0
1	B	2348	0	2379	108	0
2	E	217	0	208	6	0
2	F	136	0	124	14	0
3	A	45	0	0	0	0
3	B	26	0	0	0	0
3	E	6	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4962	0	4915	202	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 21.

All (202) 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:B:205:LYS:HE2	1:B:214:ILE:HG13	1.37	1.04
1:B:182:LEU:HD23	1:B:290:VAL:HB	1.36	1.02
1:A:275:ASN:H	1:A:279:GLN:HE22	1.03	1.01
1:B:56:LYS:HG3	1:B:115:ILE:HG13	1.40	0.99
1:B:230:ASN:HB3	1:B:232:PRO:HD2	1.45	0.98
2:F:439:ASP:HA	2:F:442:THR:HB	1.48	0.95
1:A:38:GLU:HG3	1:A:39:SER:N	1.84	0.90
2:F:432:GLU:HG3	2:F:433:ASP:H	1.41	0.84
1:A:38:GLU:HG3	1:A:39:SER:H	1.41	0.84
1:B:298:LYS:HE2	2:F:430:LEU:HD22	1.62	0.81
1:A:275:ASN:N	1:A:279:GLN:HE22	1.79	0.81
1:B:342:LEU:HD23	2:F:443:GLN:OE1	1.81	0.79
1:A:38:GLU:CG	1:A:39:SER:N	2.46	0.78
1:A:207:ARG:NH2	1:A:354:GLU:OE1	2.19	0.76
1:A:111:GLU:OE1	1:A:355:VAL:HG13	1.88	0.73
1:B:56:LYS:CG	1:B:115:ILE:HG13	2.16	0.73
2:F:439:ASP:HA	2:F:442:THR:CB	2.18	0.73
1:A:107:ARG:NH2	1:A:359:ALA:O	2.22	0.72
2:E:423:LYS:HD2	2:E:426:GLU:HG3	1.71	0.72
1:B:291:PHE:HB2	1:B:333:PHE:CD2	2.25	0.71
1:A:276:HIS:H	1:A:279:GLN:NE2	1.88	0.71
1:B:177:MET:H	1:B:261:ALA:HB1	1.56	0.71
1:B:184:GLY:HA3	1:B:193:THR:HG23	1.72	0.70
1:B:133:GLN:C	1:B:135:ALA:H	1.96	0.69
1:A:93:LEU:CD2	1:A:108:LEU:HD23	2.23	0.68
1:A:247:ILE:O	1:A:247:ILE:HG12	1.92	0.68
1:A:275:ASN:H	1:A:279:GLN:NE2	1.85	0.68
1:B:351:GLU:O	1:B:355:VAL:HG23	1.93	0.67
2:F:435:LYS:HA	2:F:438:LEU:HB2	1.77	0.67
1:A:107:ARG:HD2	1:A:113:GLY:O	1.96	0.66
1:A:55:ALA:HA	1:A:58:LYS:HG3	1.77	0.66
1:B:323:ASP:O	1:B:327:GLN:HG3	1.96	0.66
1:B:51:GLN:NE2	1:B:54:ARG:HH21	1.94	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:GLU:HG3	1:B:345:ALA:CA	2.27	0.65
1:B:50:GLN:O	1:B:54:ARG:HG3	1.96	0.65
1:A:38:GLU:O	1:A:41:ARG:HB3	1.97	0.65
1:A:302:ARG:HG3	1:A:302:ARG:HH11	1.62	0.64
1:B:204:LEU:HD11	1:B:349:LEU:HD21	1.79	0.64
1:B:322:TYR:CZ	1:B:326:VAL:HG21	2.34	0.63
1:A:247:ILE:O	1:A:251:GLN:HG3	1.98	0.63
1:B:204:LEU:HD21	1:B:349:LEU:HD23	1.81	0.63
1:B:286:ALA:N	1:B:287:PRO:HD3	2.13	0.62
1:A:187:LEU:HG	1:A:321:ALA:CB	2.29	0.62
1:B:172:ASP:HB3	1:B:226:ARG:NH2	2.15	0.62
1:A:93:LEU:HD23	1:A:108:LEU:HD23	1.82	0.62
1:B:185:PRO:HG3	1:B:196:MET:CE	2.30	0.62
1:B:238:ILE:O	1:B:241:SER:HB3	1.99	0.62
1:B:129:LEU:C	1:B:131:GLN:H	2.03	0.62
1:B:214:ILE:CG2	1:B:268:VAL:HB	2.30	0.62
1:B:214:ILE:N	1:B:214:ILE:HD13	2.15	0.61
1:B:180:VAL:HB	1:B:268:VAL:HA	1.81	0.61
1:A:127:ILE:O	1:A:131:GLN:HG3	2.01	0.61
1:B:185:PRO:HD2	1:B:193:THR:HG23	1.83	0.61
1:B:231:ASN:N	1:B:232:PRO:HD2	2.15	0.61
2:F:431:GLU:HA	2:F:434:LEU:HB2	1.83	0.60
1:B:184:GLY:CA	1:B:197:GLN:HE21	2.14	0.60
1:A:50:GLN:O	1:A:54:ARG:HD3	2.02	0.60
2:E:442:THR:HA	2:E:445:GLU:HG3	1.83	0.60
1:B:339:GLU:HG3	1:B:345:ALA:HA	1.83	0.59
1:B:296:SER:HB3	1:B:298:LYS:HG2	1.84	0.59
1:A:312:MET:HE3	1:A:315:LEU:HD22	1.83	0.58
1:B:51:GLN:NE2	1:B:54:ARG:NH2	2.51	0.58
1:A:191:GLU:O	1:A:195:MET:HG3	2.04	0.58
1:B:214:ILE:HG22	1:B:268:VAL:HB	1.86	0.58
1:B:173:VAL:O	1:B:226:ARG:NH2	2.36	0.58
1:A:339:GLU:H	1:A:339:GLU:CD	2.05	0.58
1:A:187:LEU:HG	1:A:321:ALA:HB2	1.85	0.57
1:B:205:LYS:HE2	1:B:214:ILE:CG1	2.26	0.57
1:B:133:GLN:HG2	1:B:134:LYS:N	2.19	0.56
1:B:182:LEU:HD12	1:B:201:PHE:CE2	2.40	0.56
1:B:203:PHE:CE1	1:B:346:CYS:HB3	2.41	0.56
1:B:203:PHE:CZ	1:B:346:CYS:HB3	2.41	0.56
1:B:49:GLN:O	1:B:53:GLU:HG2	2.06	0.55
1:A:182:LEU:HD23	1:A:290:VAL:HB	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:VAL:O	1:B:183:VAL:HG23	2.07	0.54
1:A:128:ARG:NH1	1:A:129:LEU:HD11	2.23	0.54
1:B:231:ASN:H	1:B:232:PRO:HD2	1.72	0.54
1:A:93:LEU:HD21	1:A:108:LEU:HD23	1.88	0.54
1:B:182:LEU:HD23	1:B:290:VAL:CB	2.23	0.54
1:B:184:GLY:H	1:B:197:GLN:NE2	2.06	0.54
1:B:53:GLU:HA	1:B:56:LYS:HD3	1.90	0.54
1:A:71:CYS:SG	1:A:73:VAL:HG12	2.48	0.54
1:B:307:ARG:HB3	1:B:311:GLN:HG3	1.90	0.53
1:B:196:MET:HE1	1:B:294:VAL:HG21	1.91	0.53
1:B:185:PRO:HG3	1:B:196:MET:HE3	1.90	0.53
1:A:302:ARG:HG3	1:A:302:ARG:NH1	2.23	0.53
1:B:83:SER:O	1:B:116:ALA:HB1	2.08	0.53
1:A:55:ALA:O	1:A:96:LYS:HE3	2.08	0.53
1:B:230:ASN:HB3	1:B:232:PRO:CD	2.31	0.53
1:B:109:VAL:CG1	1:B:360:THR:HG22	2.38	0.53
1:A:255:GLU:CD	1:B:235:ARG:HH22	2.13	0.52
1:B:277:PRO:HB3	1:B:289:ILE:HD13	1.92	0.52
2:F:432:GLU:HG3	2:F:433:ASP:N	2.17	0.52
1:A:340:ASN:HD22	1:A:340:ASN:C	2.14	0.51
1:B:56:LYS:HG3	1:B:115:ILE:CG1	2.28	0.51
1:B:357:TRP:O	1:B:361:HIS:HB2	2.09	0.51
1:B:183:VAL:O	1:B:184:GLY:O	2.29	0.51
1:B:201:PHE:HE1	1:B:270:ASP:OD1	1.94	0.51
1:B:43:GLU:HA	1:B:43:GLU:OE1	2.11	0.51
1:B:185:PRO:HG3	1:B:196:MET:HE2	1.92	0.51
1:A:173:VAL:HG11	1:B:235:ARG:HG2	1.93	0.50
1:B:184:GLY:N	1:B:197:GLN:NE2	2.59	0.50
1:A:224:ALA:HB2	1:A:254:ILE:HD11	1.92	0.50
1:B:263:SER:O	1:B:264:LEU:HB2	2.10	0.50
1:A:199:ALA:HB2	2:E:444:ALA:HB2	1.94	0.49
1:B:204:LEU:HD21	1:B:349:LEU:CD2	2.42	0.49
1:B:231:ASN:N	1:B:232:PRO:CD	2.75	0.49
1:A:304:ILE:HD12	1:A:319:MET:HE3	1.93	0.49
1:B:206:HIS:HA	1:B:209:ASP:HB2	1.94	0.49
1:A:87:PHE:HB3	1:A:108:LEU:HD21	1.95	0.49
1:B:288:ILE:HA	1:B:334:ASP:OD2	2.13	0.49
1:B:73:VAL:HG23	1:B:86:ASN:HD21	1.78	0.48
1:A:276:HIS:ND1	1:A:277:PRO:HD2	2.28	0.48
1:B:107:ARG:HD2	1:B:113:GLY:O	2.14	0.48
1:B:172:ASP:HB3	1:B:226:ARG:CZ	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:GLN:HA	1:B:134:LYS:HB2	1.95	0.48
1:B:133:GLN:C	1:B:135:ALA:N	2.65	0.48
1:A:341:GLN:HB2	1:A:344:ASP:OD2	2.14	0.48
2:F:437:TYR:O	2:F:441:ILE:HG13	2.13	0.48
1:A:49:GLN:O	1:A:53:GLU:HG3	2.13	0.47
2:E:425:ARG:HG3	2:E:425:ARG:O	2.14	0.47
2:F:439:ASP:CA	2:F:442:THR:HB	2.33	0.47
1:A:276:HIS:N	1:A:279:GLN:NE2	2.59	0.47
1:B:239:GLU:C	1:B:241:SER:H	2.18	0.47
1:A:38:GLU:HG2	1:A:40:ALA:H	1.80	0.47
1:A:257:ILE:HD13	1:A:269:LEU:HD11	1.96	0.47
1:B:214:ILE:HG23	1:B:268:VAL:HB	1.96	0.47
1:B:203:PHE:CE1	1:B:350:ALA:HB2	2.50	0.47
1:A:247:ILE:O	1:A:247:ILE:CG1	2.61	0.47
1:A:220:ASP:OD1	1:A:223:LEU:HG	2.15	0.47
1:A:43:GLU:OE2	1:A:47:GLN:HG3	2.15	0.47
1:B:275:ASN:O	1:B:325:LEU:HD21	2.14	0.46
1:A:38:GLU:N	1:A:41:ARG:HD3	2.30	0.46
1:B:184:GLY:CA	1:B:197:GLN:NE2	2.79	0.46
1:B:214:ILE:H	1:B:214:ILE:HD13	1.79	0.46
1:A:203:PHE:CE2	1:A:207:ARG:HG3	2.51	0.46
1:A:186:SER:OG	1:A:187:LEU:N	2.49	0.46
1:A:85:VAL:HG22	1:A:86:ASN:N	2.31	0.46
1:A:128:ARG:HH12	1:A:129:LEU:HD11	1.81	0.46
1:A:79:PRO:HD3	1:A:103:TRP:CE2	2.51	0.46
1:A:193:THR:O	1:A:197:GLN:HG3	2.16	0.45
1:B:169:PRO:HA	1:B:170:PRO:HD3	1.85	0.45
1:A:185:PRO:HB3	1:A:294:VAL:HG23	1.99	0.45
1:A:123:ARG:O	1:A:123:ARG:HG3	2.15	0.45
1:A:312:MET:CE	1:A:315:LEU:HD22	2.47	0.45
2:F:438:LEU:O	2:F:442:THR:N	2.46	0.45
1:A:128:ARG:NH1	1:A:129:LEU:CD1	2.80	0.45
1:B:184:GLY:H	1:B:197:GLN:HE22	1.63	0.45
1:B:129:LEU:O	1:B:131:GLN:N	2.50	0.44
2:E:441:ILE:O	2:E:445:GLU:HG3	2.17	0.44
1:A:89:ALA:O	1:A:90:LYS:HB2	2.16	0.44
1:A:211:ARG:HB2	1:A:357:TRP:CH2	2.52	0.44
1:A:300:LEU:HG	1:A:319:MET:HE1	2.00	0.44
1:B:175:PRO:HG3	1:B:258:PHE:CE1	2.52	0.44
1:A:325:LEU:O	1:A:328:CYS:HB2	2.16	0.44
2:F:440:TRP:C	2:F:440:TRP:CD1	2.91	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:SER:O	1:A:116:ALA:HB1	2.18	0.43
1:B:186:SER:HB3	1:B:193:THR:OG1	2.18	0.43
1:B:276:HIS:ND1	1:B:277:PRO:HD2	2.32	0.43
1:B:236:THR:O	1:B:240:ARG:HG2	2.18	0.43
1:B:347:GLU:O	1:B:351:GLU:HB3	2.18	0.43
2:E:444:ALA:C	2:E:446:ASP:H	2.20	0.43
1:A:205:LYS:HB2	1:A:205:LYS:HE3	1.74	0.43
1:B:331:GLU:O	1:B:333:PHE:N	2.51	0.43
1:A:347:GLU:O	1:A:351:GLU:HG3	2.19	0.43
1:A:56:LYS:HA	1:A:115:ILE:HD12	2.00	0.43
1:B:129:LEU:C	1:B:131:GLN:N	2.71	0.43
1:B:182:LEU:CD1	1:B:197:GLN:HG2	2.47	0.43
1:B:40:ALA:O	1:B:43:GLU:HB3	2.18	0.43
1:A:214:ILE:HG12	1:A:268:VAL:HB	2.00	0.43
1:B:191:GLU:HG3	1:B:311:GLN:NE2	2.34	0.43
1:B:317:VAL:HA	1:B:320:MET:CE	2.49	0.43
1:B:70:TYR:HB3	1:B:87:PHE:CZ	2.54	0.43
1:A:168:VAL:HA	1:A:169:PRO:HD3	1.80	0.42
1:A:340:ASN:HD22	1:A:341:GLN:N	2.17	0.42
1:B:240:ARG:HB3	1:B:240:ARG:HE	1.61	0.42
1:A:107:ARG:HB3	1:A:115:ILE:HA	2.01	0.42
1:A:304:ILE:HD12	1:A:319:MET:CE	2.49	0.42
1:A:174:VAL:HB	1:A:175:PRO:CD	2.49	0.42
1:B:233:GLY:O	1:B:237:ILE:HG13	2.20	0.42
1:B:51:GLN:HE21	1:B:54:ARG:NH2	2.17	0.42
1:B:317:VAL:HA	1:B:320:MET:HE2	2.01	0.42
1:A:275:ASN:N	1:A:279:GLN:NE2	2.57	0.41
1:B:211:ARG:HB2	1:B:357:TRP:CH2	2.55	0.41
1:B:244:ARG:HA	1:B:244:ARG:HD2	1.81	0.41
1:B:295:SER:O	1:B:322:TYR:OH	2.36	0.41
1:B:203:PHE:CE2	1:B:346:CYS:HB3	2.56	0.41
1:A:78:CYS:HA	1:A:103:TRP:CZ2	2.55	0.41
1:A:305:ARG:HG2	1:A:312:MET:HE2	2.01	0.41
1:A:174:VAL:HG12	1:A:284:SER:O	2.19	0.41
1:B:262:LYS:HE2	1:B:262:LYS:HB3	1.82	0.41
1:B:294:VAL:HG22	2:F:437:TYR:CE2	2.56	0.41
1:A:125:GLU:OE2	1:A:128:ARG:NH1	2.53	0.41
1:B:38:GLU:HG3	1:B:38:GLU:O	2.18	0.41
1:B:214:ILE:HA	1:B:268:VAL:O	2.20	0.41
1:B:203:PHE:CD1	1:B:346:CYS:HB3	2.56	0.41
1:B:193:THR:O	1:B:197:GLN:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ILE:HG22	1:B:128:ARG:N	2.35	0.41
2:F:430:LEU:N	2:F:432:GLU:HG2	2.36	0.41
1:A:203:PHE:CZ	1:A:207:ARG:HG3	2.56	0.41
1:A:253:GLU:OE1	1:A:253:GLU:HA	2.21	0.40
1:A:250:VAL:O	1:A:254:ILE:HG12	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	A	268/351 (76%)	255 (95%)	13 (5%)	0	100	100
1	B	291/351 (83%)	265 (91%)	20 (7%)	6 (2%)	7	13
2	E	23/25 (92%)	21 (91%)	2 (9%)	0	100	100
2	F	15/25 (60%)	12 (80%)	2 (13%)	1 (7%)	1	1
All	All	597/752 (79%)	553 (93%)	37 (6%)	7 (1%)	13	27

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	362	HIS
1	B	184	GLY
1	B	332	SER
1	B	130	LYS
1	B	191	GLU
1	B	134	LYS
2	F	445	GLU

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	242/310 (78%)	237 (98%)	5 (2%)	53	77
1	B	261/310 (84%)	242 (93%)	19 (7%)	14	28
2	E	23/23 (100%)	18 (78%)	5 (22%)	1	1
2	F	14/23 (61%)	10 (71%)	4 (29%)	0	0
All	All	540/666 (81%)	507 (94%)	33 (6%)	18	38

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	123	ARG
1	A	133	GLN
1	A	207	ARG
1	A	284	SER
1	A	340	ASN
1	B	52	LEU
1	B	108	LEU
1	B	133	GLN
1	B	187	LEU
1	B	196	MET
1	B	197	GLN
1	B	206	HIS
1	B	214	ILE
1	B	226	ARG
1	B	228	VAL
1	B	240	ARG
1	B	241	SER
1	B	244	ARG
1	B	245	SER
1	B	246	SER
1	B	296	SER
1	B	306	SER
1	B	351	GLU
1	B	362	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	422	GLN
2	E	423	LYS
2	E	425	ARG
2	E	442	THR
2	E	446	ASP
2	F	434	LEU
2	F	438	LEU
2	F	439	ASP
2	F	440	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	GLN
1	A	122	GLN
1	A	279	GLN
1	A	301	GLN
1	A	327	GLN
1	A	340	ASN
1	A	361	HIS
1	B	50	GLN
1	B	51	GLN
1	B	57	HIS
1	B	197	GLN
1	B	206	HIS
1	B	231	ASN
1	B	265	GLN
1	B	311	GLN
2	E	429	GLN
2	E	443	GLN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	274/351 (78%)	-0.09	13 (4%) 31 25	20, 38, 89, 122	0
1	B	295/351 (84%)	0.02	12 (4%) 37 30	32, 55, 90, 119	0
2	E	25/25 (100%)	-0.11	0 100 100	21, 40, 76, 84	0
2	F	17/25 (68%)	1.07	4 (23%) 0 0	57, 82, 121, 121	0
All	All	611/752 (81%)	-0.01	29 (4%) 31 25	20, 47, 90, 122	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	GLN	5.0
1	B	363	PRO	4.3
1	B	135	ALA	3.8
1	B	167	HIS	3.6
1	A	43	GLU	3.5
1	B	39	SER	3.4
1	A	42	ARG	3.4
1	A	39	SER	3.3
2	F	435	LYS	3.3
1	A	167	HIS	3.3
2	F	431	GLU	3.0
1	A	41	ARG	3.0
2	F	434	LEU	2.7
1	B	133	GLN	2.7
1	B	42	ARG	2.6
1	A	40	ALA	2.5
2	F	439	ASP	2.5
1	B	57	HIS	2.5
1	B	41	ARG	2.5
1	B	362	HIS	2.4
1	A	134	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	129	LEU	2.3
1	B	206	HIS	2.2
1	A	246	SER	2.1
1	A	247	ILE	2.1
1	B	292	VAL	2.1
1	A	38	GLU	2.1
1	A	46	SER	2.0
1	B	111	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 carbohydrates 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.