WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 10:28 AM EDT

PDB ID : 3BE1

Title : Dual specific bH1 Fab in complex with the extracellular domain of HER2/ErbB-2

Authors : Bostrom, J.M.; Wiesmann, C.; Appleton, B.A.

Deposited on : 2007-11-15

Resolution : 2.90 Å(reported)

The following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
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)	:	2.35

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 2.90 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	Percentile Ranks	Value
Rfree		0.283
Clashscore		8
Ramachandran outliers		1.4%
Sidechain outliers		3.3%
RSRZ outliers		11.7%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
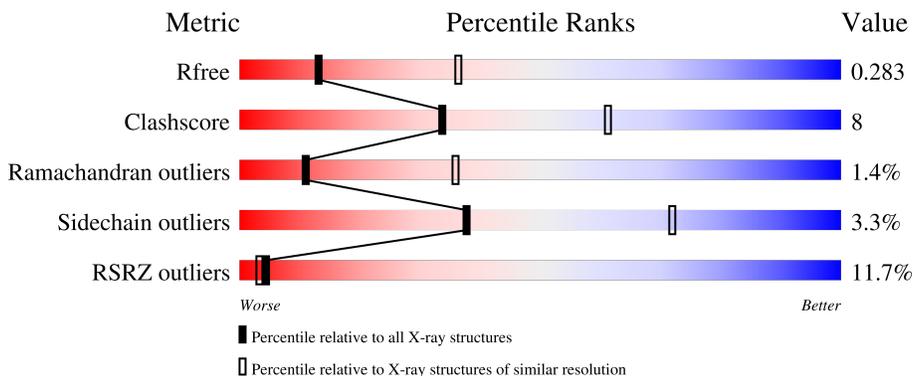
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	624	2% / 77% / 16% / 7%
2	H	230	27% / 75% / 17% / 7%
3	L	218	20% / 75% / 22%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 7810 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 Receptor tyrosine-protein kinase erbB-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	583	Total	C	N	O	S	0	0	0
			4501	2800	807	842	52			

- Molecule 2 is a protein called Fab Fragment-Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	213	Total	C	N	O	S	0	0	0
			1605	1018	270	311	6			

- Molecule 3 is a protein called Fab Fragment-Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	216	Total	C	N	O	S	0	0	0
			1664	1048	276	335	5			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
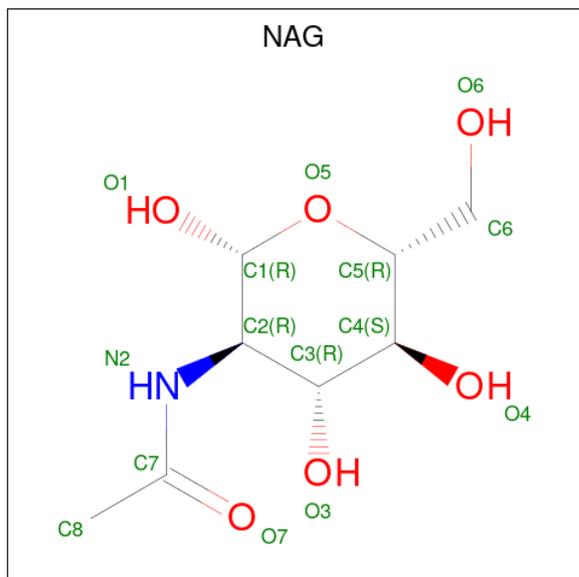
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total C N O				0	0
			14 8 1 5					
4	A	1	Total C N O				0	0
			14 8 1 5					

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).

MES

O1

C2 O C6

C3 C5

H
N+ N4

C7

C8

O2S O S O O1S

O−

O3S
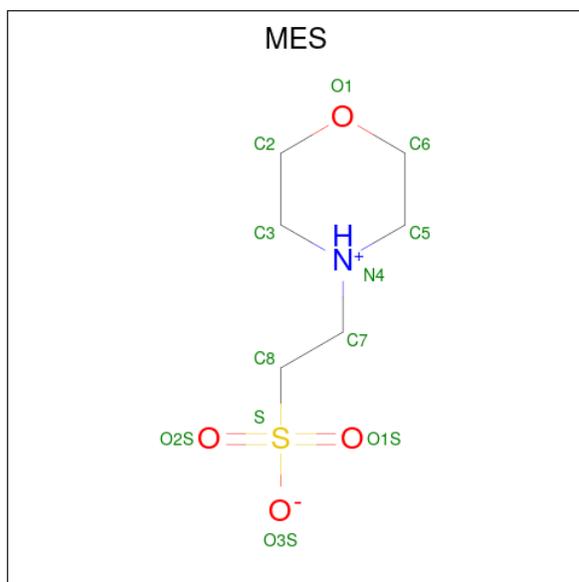
| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	L	1	Total C N O S					0	0
			12 6 1 4 1						

3 Residue-property plots ⓘ

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: Receptor tyrosine-protein kinase erbB-2
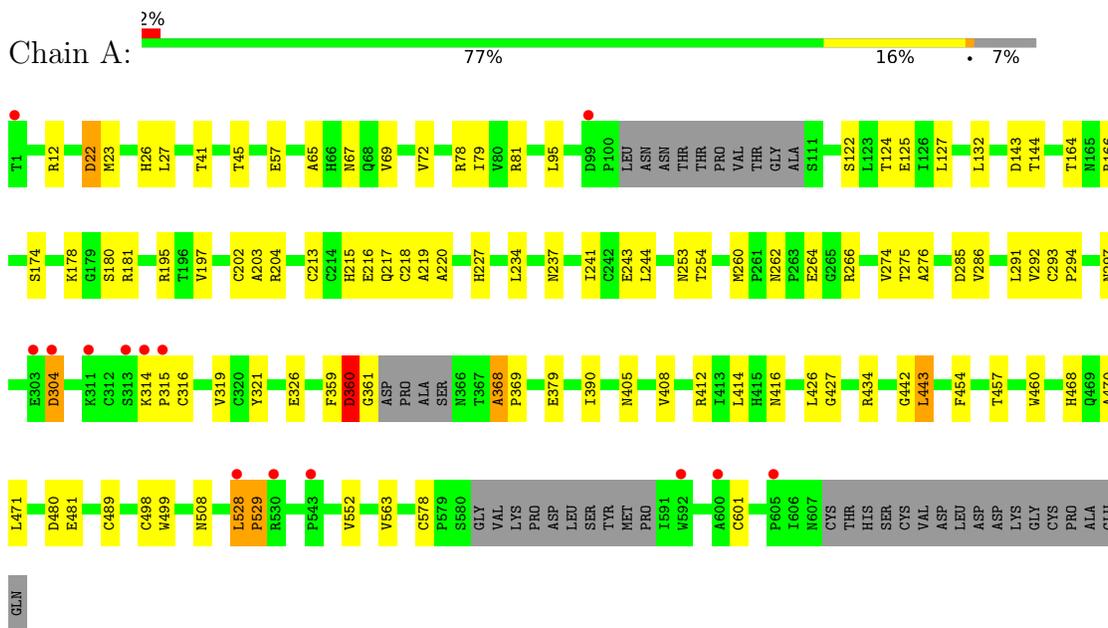
• Molecule 2: Fab Fragment-Heavy Chain
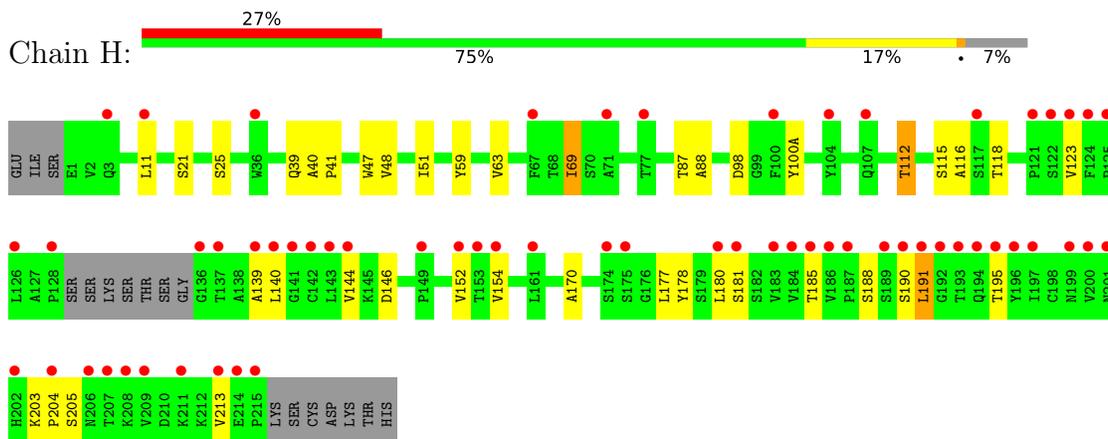
• Molecule 3: Fab Fragment-Light Chain
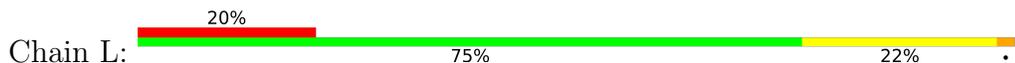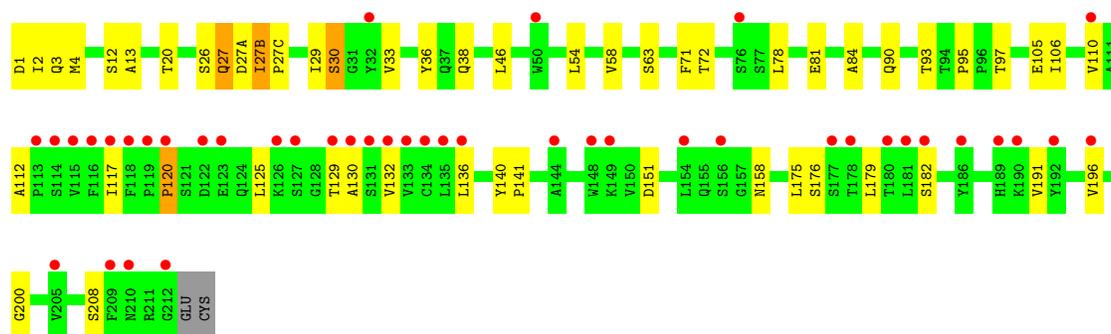
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	62.32Å 115.06Å 208.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.90 48.49 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.8 (30.00-2.90) 99.3 (48.49-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.91Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.236 , 0.277 0.220 , 0.283	Depositor DCC
R_{free} test set	1715 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	58.6	Xtriage
Anisotropy	0.701	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 66.8	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7810	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 ⓘ

5.1 Standard geometry ⓘ

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

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	0.52	1/4607 (0.0%)	0.66	0/6266
2	H	0.35	0/1646	0.52	0/2245
3	L	0.36	0/1705	0.51	0/2320
All	All	0.46	1/7958 (0.0%)	0.60	0/10831

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	CYS	CB-SG	-5.09	1.73	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	427	GLY	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4501	0	4308	73	0
2	H	1605	0	1562	23	0
3	L	1664	0	1608	32	0
4	A	28	0	26	5	0
5	L	12	0	12	1	0
All	All	7810	0	7516	127	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 8.

All (127) 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:237:ASN:HD21	4:A:1001:NAG:C1	1.21	1.53
1:A:508:ASN:HD21	4:A:1002:NAG:C1	1.34	1.38
1:A:124:THR:HG21	1:A:220:ALA:O	1.45	1.14
1:A:578:CYS:HG	1:A:601:CYS:HG	0.98	0.93
1:A:144:THR:HG22	1:A:181:ARG:HA	1.49	0.91
1:A:143:ASP:HB3	1:A:164:THR:HG21	1.59	0.84
1:A:125:GLU:OE1	1:A:219:ALA:O	1.96	0.83
1:A:237:ASN:HD21	4:A:1001:NAG:C2	1.91	0.82
1:A:124:THR:CG2	1:A:220:ALA:O	2.33	0.74
1:A:274:VAL:CG1	1:A:276:ALA:O	2.35	0.74
1:A:72:VAL:O	1:A:72:VAL:HG23	1.90	0.72
1:A:359:PHE:O	1:A:361:GLY:N	2.25	0.70
1:A:195:ARG:HG3	1:A:203:ALA:O	1.93	0.69
1:A:144:THR:CG2	1:A:181:ARG:HA	2.21	0.68
2:H:139:ALA:HB2	2:H:185:THR:HG22	1.74	0.68
1:A:294:PRO:O	1:A:297:ASN:ND2	2.28	0.67
1:A:368:ALA:HB1	1:A:369:PRO:CD	2.26	0.66
3:L:120:PRO:HD3	3:L:132:VAL:HG22	1.78	0.66
1:A:443:LEU:HD23	1:A:470:ALA:O	1.98	0.64
3:L:136:LEU:HD21	3:L:196:VAL:CG1	2.27	0.63
1:A:217:GLN:HE22	1:A:244:LEU:N	1.97	0.63
2:H:140:LEU:HD13	2:H:213:VAL:HG21	1.81	0.63
1:A:143:ASP:HB3	1:A:164:THR:CG2	2.27	0.62
3:L:175:LEU:HD23	3:L:176:SER:N	2.14	0.61
3:L:117:ILE:HG21	3:L:208:SER:HA	1.83	0.61
2:H:48:VAL:HG13	2:H:63:VAL:HG11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:GLN:NE2	1:A:244:LEU:N	2.50	0.59
1:A:457:THR:HG23	1:A:498:CYS:O	2.02	0.59
3:L:97:THR:HG22	5:L:215:MES:O3S	2.02	0.59
1:A:454:PHE:C	1:A:457:THR:HG22	2.24	0.58
1:A:253:ASN:HB2	1:A:260:MET:HE3	1.86	0.57
1:A:457:THR:OG1	1:A:489:CYS:SG	2.62	0.57
1:A:197:VAL:HG13	1:A:197:VAL:O	2.04	0.57
3:L:125:LEU:HD23	3:L:130:ALA:HB2	1.87	0.56
1:A:237:ASN:CG	4:A:1001:NAG:C1	2.73	0.55
1:A:253:ASN:HD22	1:A:260:MET:HE1	1.71	0.55
1:A:274:VAL:HG12	1:A:276:ALA:O	2.07	0.55
1:A:195:ARG:HB2	1:A:204:ARG:NH1	2.22	0.54
1:A:241:ILE:HG22	1:A:243:GLU:HG3	1.89	0.54
1:A:253:ASN:HD22	1:A:260:MET:CE	2.21	0.54
3:L:129:THR:HG22	3:L:182:SER:CB	2.37	0.53
1:A:414:LEU:HD22	1:A:442:GLY:HA3	1.91	0.53
1:A:274:VAL:HG11	1:A:276:ALA:O	2.09	0.51
3:L:136:LEU:HD21	3:L:196:VAL:HG11	1.91	0.51
1:A:95:LEU:HD21	1:A:132:LEU:CD2	2.41	0.51
3:L:129:THR:HG22	3:L:182:SER:HB2	1.90	0.51
1:A:72:VAL:O	1:A:72:VAL:CG2	2.58	0.51
2:H:87:THR:HG23	2:H:112:THR:HA	1.90	0.51
2:H:140:LEU:HB2	2:H:213:VAL:HG11	1.92	0.51
2:H:146:ASP:HB3	2:H:177:LEU:HD13	1.92	0.51
1:A:41:THR:HA	1:A:65:ALA:O	2.12	0.50
1:A:508:ASN:HD22	4:A:1002:NAG:C1	2.17	0.49
1:A:217:GLN:HE21	1:A:243:GLU:HA	1.76	0.49
1:A:22:ASP:N	1:A:22:ASP:OD1	2.45	0.49
1:A:262:ASN:OD1	1:A:264:GLU:N	2.43	0.49
1:A:219:ALA:HB2	1:A:234:LEU:CA	2.43	0.49
2:H:47:TRP:CH2	3:L:95:PRO:HB3	2.47	0.49
1:A:219:ALA:HB2	1:A:234:LEU:HA	1.95	0.48
3:L:158:ASN:OD1	3:L:179:LEU:HD11	2.14	0.48
1:A:12:ARG:NH1	1:A:416:ASN:OD1	2.47	0.48
1:A:217:GLN:HE22	1:A:244:LEU:CA	2.26	0.48
2:H:180:LEU:HD12	2:H:181:SER:N	2.29	0.48
3:L:110:VAL:HG12	3:L:141:PRO:HD3	1.96	0.48
1:A:379:GLU:O	1:A:405:ASN:ND2	2.39	0.48
1:A:360:ASP:O	1:A:361:GLY:C	2.52	0.48
1:A:368:ALA:HB1	1:A:369:PRO:HD2	1.95	0.48
3:L:2:ILE:HD13	3:L:29:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:LEU:HD22	1:A:412:ARG:HB3	1.96	0.47
1:A:552:VAL:O	1:A:563:VAL:HG21	2.14	0.47
2:H:203:LYS:N	2:H:204:PRO:CD	2.77	0.47
1:A:67:ASN:HB3	1:A:69:VAL:HG12	1.96	0.47
2:H:39:GLN:C	2:H:88:ALA:HB1	2.36	0.47
1:A:293:CYS:HB3	1:A:297:ASN:HB2	1.98	0.46
1:A:81:ARG:HG2	1:A:127:LEU:HD12	1.98	0.46
1:A:454:PHE:HD2	1:A:457:THR:HG21	1.81	0.46
2:H:140:LEU:HD13	2:H:213:VAL:CG2	2.46	0.46
1:A:480:ASP:OD1	1:A:481:GLU:N	2.49	0.46
3:L:29:ILE:O	3:L:30:SER:C	2.53	0.46
3:L:140:TYR:CG	3:L:141:PRO:HA	2.51	0.46
3:L:136:LEU:HD21	3:L:196:VAL:HG13	1.95	0.46
3:L:12:SER:HA	3:L:105:GLU:O	2.16	0.45
3:L:117:ILE:HG21	3:L:208:SER:CA	2.47	0.45
3:L:112:ALA:HB2	3:L:200:GLY:O	2.16	0.45
2:H:59:TYR:CE1	2:H:69:ILE:HG22	2.51	0.45
3:L:20:THR:HG23	3:L:72:THR:HG23	1.99	0.45
2:H:152:VAL:HG12	2:H:154:VAL:HG23	1.98	0.44
2:H:48:VAL:CG1	2:H:63:VAL:HG11	2.48	0.44
3:L:38:GLN:O	3:L:84:ALA:HB1	2.17	0.44
2:H:123:VAL:HG22	2:H:144:VAL:HG22	1.99	0.44
1:A:27:LEU:O	1:A:468:HIS:ND1	2.47	0.44
3:L:3:GLN:HB2	3:L:26:SER:OG	2.17	0.44
3:L:13:ALA:HB3	3:L:78:LEU:HD22	1.98	0.44
2:H:188:SER:O	2:H:191:LEU:HD13	2.18	0.43
1:A:314:LYS:HB2	1:A:315:PRO:HD2	2.00	0.43
1:A:321:TYR:CE2	1:A:326:GLU:HG3	2.53	0.43
1:A:79:ILE:HG23	1:A:79:ILE:O	2.18	0.43
2:H:118:THR:HG22	2:H:205:SER:HB3	2.00	0.43
2:H:139:ALA:CB	2:H:185:THR:HG22	2.45	0.43
1:A:460:TRP:CE2	1:A:471:LEU:HD22	2.53	0.43
2:H:98:ASP:O	2:H:100(A):TYR:CZ	2.72	0.43
3:L:2:ILE:HG12	3:L:27:GLN:HB3	2.00	0.43
1:A:144:THR:O	1:A:181:ARG:NH1	2.52	0.43
3:L:90:GLN:HE22	3:L:93:THR:HG22	1.83	0.42
1:A:262:ASN:OD1	1:A:262:ASN:C	2.57	0.42
2:H:51:ILE:HB	2:H:69:ILE:HD13	2.00	0.42
3:L:78:LEU:HD21	3:L:106:ILE:HD13	2.01	0.42
2:H:40:ALA:HB1	2:H:41:PRO:HD2	2.01	0.42
1:A:22:ASP:O	1:A:26:HIS:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:4:MET:HE1	3:L:90:GLN:HB3	2.00	0.42
1:A:57:GLU:HG2	1:A:79:ILE:CG2	2.49	0.42
3:L:29:ILE:HG22	3:L:33:VAL:HG23	2.02	0.42
1:A:23:MET:HG2	1:A:443:LEU:HD13	2.02	0.41
3:L:191:VAL:O	3:L:191:VAL:HG13	2.21	0.41
1:A:304:ASP:OD1	1:A:304:ASP:N	2.53	0.41
1:A:390:ILE:HG22	1:A:426:LEU:HD21	2.01	0.41
3:L:27(B):ILE:HD13	3:L:27(B):ILE:N	2.36	0.41
3:L:36:TYR:CE2	3:L:46:LEU:HD13	2.55	0.41
1:A:286:VAL:O	1:A:286:VAL:CG1	2.68	0.41
3:L:54:LEU:HD11	3:L:58:VAL:CG1	2.50	0.41
1:A:217:GLN:NE2	1:A:243:GLU:C	2.75	0.41
1:A:528:LEU:CB	1:A:529:PRO:HD3	2.51	0.41
1:A:78:ARG:HA	1:A:122:SER:O	2.21	0.41
1:A:22:ASP:O	1:A:26:HIS:CD2	2.74	0.40
1:A:266:ARG:CZ	1:A:275:THR:HG22	2.51	0.40
1:A:434:ARG:HA	1:A:499:TRP:CD1	2.56	0.40
2:H:11:LEU:HD21	2:H:116:ALA:O	2.21	0.40
2:H:170:ALA:HB1	2:H:178:TYR:HB3	2.03	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	575/624 (92%)	523 (91%)	44 (8%)	8 (1%)	11	36
2	H	209/230 (91%)	185 (88%)	21 (10%)	3 (1%)	11	36
3	L	214/218 (98%)	191 (89%)	20 (9%)	3 (1%)	11	36
All	All	998/1072 (93%)	899 (90%)	85 (8%)	14 (1%)	11	36

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	178	LYS
1	A	213	CYS
1	A	215	HIS
1	A	360	ASP
2	H	191	LEU
1	A	45	THR
3	L	27(C)	PRO
2	H	195	THR
3	L	30	SER
3	L	151	ASP
1	A	292	VAL
2	H	190	SER
1	A	368	ALA
1	A	529	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	A	503/538 (94%)	487 (97%)	16 (3%)	39	73
2	H	175/191 (92%)	170 (97%)	5 (3%)	42	76
3	L	189/192 (98%)	181 (96%)	8 (4%)	30	63
All	All	867/921 (94%)	838 (97%)	29 (3%)	38	72

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ASP
1	A	166	ARG
1	A	174	SER
1	A	180	SER
1	A	202	CYS
1	A	216	GLU
1	A	227	HIS
1	A	254	THR
1	A	285	ASP

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Mol	Chain	Res	Type
1	A	304	ASP
1	A	316	CYS
1	A	319	VAL
1	A	360	ASP
1	A	408	VAL
1	A	443	LEU
1	A	528	LEU
2	H	21	SER
2	H	25	SER
2	H	69	ILE
2	H	112	THR
2	H	115	SER
3	L	1	ASP
3	L	27	GLN
3	L	27(A)	ASP
3	L	27(B)	ILE
3	L	63	SER
3	L	71	PHE
3	L	81	GLU
3	L	120	PRO

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	2	GLN
1	A	26	HIS
1	A	53	GLN
1	A	56	GLN
1	A	217	GLN
1	A	237	ASN
1	A	307	GLN
1	A	497	HIS
1	A	508	ASN
1	A	526	GLN
1	A	542	HIS
2	H	35	HIS
3	L	199	GLN

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)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
5	MES	L	215	-	12,12,12	2.14	1 (8%)	14,16,16	2.56	7 (50%)
4	NAG	A	1001	1	14,14,15	0.74	1 (7%)	17,19,21	1.24	2 (11%)
4	NAG	A	1002	1	14,14,15	0.59	0	17,19,21	0.89	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MES	L	215	-	-	4/6/14/14	0/1/1/1
4	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1002	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	215	MES	C8-S	-7.10	1.67	1.77
4	A	1001	NAG	O5-C1	-2.07	1.40	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	215	MES	C5-N4-C3	4.60	119.19	108.83
5	L	215	MES	C7-N4-C5	3.64	120.54	111.23
5	L	215	MES	C7-N4-C3	3.53	120.26	111.23
5	L	215	MES	O1S-S-C8	3.47	111.09	106.92
5	L	215	MES	C2-C3-N4	-3.04	105.50	110.10
5	L	215	MES	O2S-S-C8	2.93	110.44	106.92
5	L	215	MES	C6-C5-N4	-2.89	105.72	110.10
4	A	1001	NAG	C1-O5-C5	-2.27	109.12	112.19
4	A	1001	NAG	O5-C1-C2	-2.14	107.92	111.29

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1002	NAG	C8-C7-N2-C2
4	A	1002	NAG	O7-C7-N2-C2
5	L	215	MES	C7-C8-S-O3S
5	L	215	MES	C8-C7-N4-C5
5	L	215	MES	C7-C8-S-O1S
5	L	215	MES	C7-C8-S-O2S

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	215	MES	1	0
4	A	1001	NAG	3	0
4	A	1002	NAG	2	0

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(Å²)	Q<0.9
1	A	583/624 (93%)	0.20	14 (2%)	59	56	19, 41, 79, 109	0
2	H	213/230 (92%)	1.51	61 (28%)	0	0	56, 86, 141, 149	0
3	L	216/218 (99%)	1.21	43 (19%)	1	0	49, 86, 143, 148	0
All	All	1012/1072 (94%)	0.69	118 (11%)	4	3	19, 59, 135, 149	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	140	LEU	11.9
2	H	184	VAL	9.2
2	H	125	PRO	8.5
3	L	181	LEU	8.4
1	A	528	LEU	8.3
2	H	213	VAL	7.6
3	L	131	SER	7.6
2	H	194	GLN	7.3
2	H	193	THR	7.2
2	H	187	PRO	6.8
2	H	143	LEU	6.6
1	A	592	TRP	6.5
2	H	123	VAL	6.3
2	H	201	ASN	6.3
3	L	117	ILE	6.2
2	H	190	SER	6.1
2	H	139	ALA	6.1
2	H	141	GLY	6.0
3	L	118	PHE	5.8
3	L	115	VAL	5.7
3	L	192	TYR	5.7
3	L	122	ASP	5.5
3	L	133	VAL	5.4

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Mol	Chain	Res	Type	RSRZ
3	L	132	VAL	5.2
3	L	178	THR	5.2
2	H	196	TYR	5.2
2	H	124	PHE	5.2
2	H	126	LEU	5.1
2	H	200	VAL	5.0
3	L	148	TRP	5.0
2	H	185	THR	5.0
3	L	182	SER	4.9
3	L	135	LEU	4.8
2	H	197	ILE	4.7
2	H	186	VAL	4.6
2	H	71	ALA	4.5
3	L	186	TYR	4.5
3	L	196	VAL	4.4
1	A	1	THR	4.2
2	H	208	LYS	4.2
3	L	119	PRO	4.0
3	L	116	PHE	4.0
2	H	137	THR	4.0
3	L	127	SER	3.8
2	H	192	GLY	3.7
3	L	113	PRO	3.7
1	A	314	LYS	3.7
1	A	313	SER	3.7
3	L	136	LEU	3.6
3	L	114	SER	3.6
2	H	142	CYS	3.5
2	H	215	PRO	3.4
2	H	174	SER	3.4
1	A	311	LYS	3.4
2	H	144	VAL	3.4
3	L	190	LYS	3.3
3	L	123	GLU	3.2
2	H	152	VAL	3.2
3	L	134	CYS	3.2
2	H	36	TRP	3.2
2	H	122	SER	3.2
3	L	129	THR	3.1
2	H	183	VAL	3.0
2	H	154	VAL	3.0
1	A	303	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
2	H	209	VAL	2.9
1	A	315	PRO	2.8
2	H	214	GLU	2.8
2	H	175	SER	2.8
3	L	177	SER	2.8
2	H	128	PRO	2.8
3	L	144	ALA	2.8
2	H	181	SER	2.8
3	L	189	HIS	2.8
2	H	195	THR	2.8
3	L	76	SER	2.8
2	H	202	HIS	2.8
2	H	207	THR	2.7
3	L	205	VAL	2.7
2	H	11	LEU	2.7
3	L	209	PHE	2.7
2	H	136	GLY	2.7
1	A	543	PRO	2.6
2	H	77	THR	2.6
2	H	189	SER	2.6
3	L	32	TYR	2.6
1	A	530	ARG	2.6
3	L	126	LYS	2.6
3	L	180	THR	2.6
2	H	180	LEU	2.6
3	L	156	SER	2.6
3	L	50	TRP	2.6
1	A	605	PRO	2.5
3	L	210	ASN	2.5
2	H	204	PRO	2.4
2	H	100	PHE	2.4
2	H	153	THR	2.4
3	L	154	LEU	2.4
2	H	211	LYS	2.4
3	L	212	GLY	2.3
1	A	304	ASP	2.3
2	H	117	SER	2.3
3	L	130	ALA	2.3
2	H	199	ASN	2.3
3	L	149	LYS	2.3
1	A	600	ALA	2.3
2	H	107	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
3	L	120	PRO	2.2
2	H	67	PHE	2.2
1	A	99	ASP	2.2
3	L	110	VAL	2.2
2	H	3	GLN	2.1
2	H	104	TYR	2.1
2	H	206	ASN	2.1
2	H	121	PRO	2.1
2	H	191	LEU	2.1
2	H	149	PRO	2.0
2	H	161	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
4	NAG	A	1002	14/15	0.73	0.36	107,113,123,125	0
4	NAG	A	1001	14/15	0.90	0.22	28,46,49,49	0
5	MES	L	215	12/12	0.93	0.21	76,91,99,100	0

6.5 Other polymers ⓘ

There are no such residues in this entry.