Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 06:10 PM BST

PDB ID	:	4QFL
Title	:	Crystal structure of dipeptide binding protein from pseudoalteromonas sp. SM9913 in complex with Ala-Phe
Authors	:	Li, C.Y.; Zhang, Y.Z.
Deposited on	:	2014-05-21
Resolution	:	1.75 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:

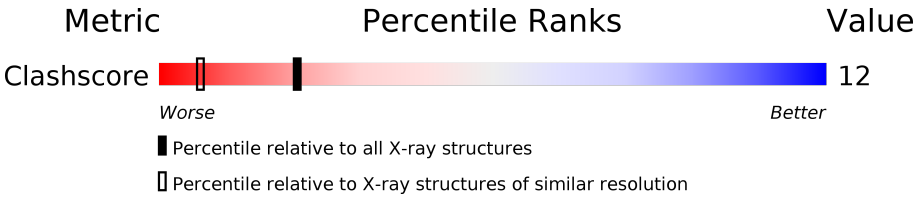
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4.dev1

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 1.75 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))
Clashscore	141614	3923 (1.76-1.72)

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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	541	71% 23% 6%
1	B	541	71% 22% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8932 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.

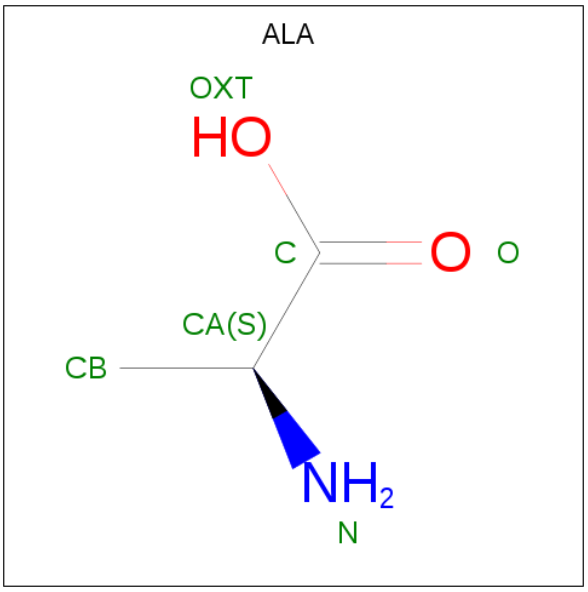
- Molecule 1 is a protein called ABC transporter periplasmic peptide-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	507	Total	C	N	O	S	0	2	0
			4098	2628	691	765	14			
1	B	507	Total	C	N	O	S	0	3	0
			4102	2629	692	767	14			

There are 12 discrepancies between the modelled and reference sequences:

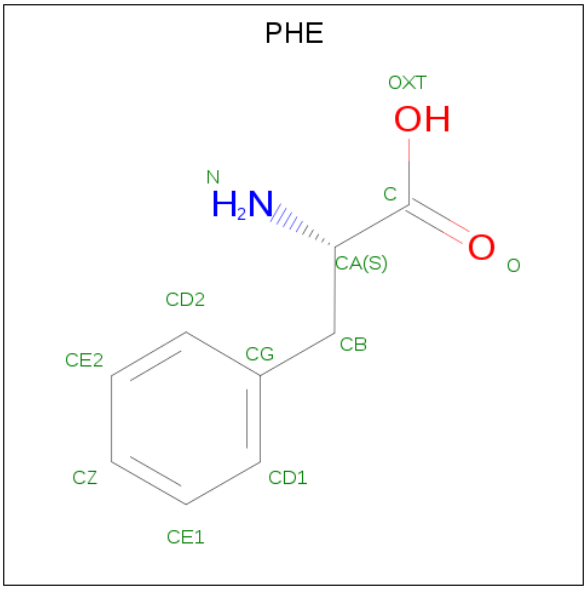
Chain	Residue	Modelled	Actual	Comment	Reference
A	536	HIS	-	EXPRESSION TAG	UNP A7Y7W1
A	537	HIS	-	EXPRESSION TAG	UNP A7Y7W1
A	538	HIS	-	EXPRESSION TAG	UNP A7Y7W1
A	539	HIS	-	EXPRESSION TAG	UNP A7Y7W1
A	540	HIS	-	EXPRESSION TAG	UNP A7Y7W1
A	541	HIS	-	EXPRESSION TAG	UNP A7Y7W1
B	536	HIS	-	EXPRESSION TAG	UNP A7Y7W1
B	537	HIS	-	EXPRESSION TAG	UNP A7Y7W1
B	538	HIS	-	EXPRESSION TAG	UNP A7Y7W1
B	539	HIS	-	EXPRESSION TAG	UNP A7Y7W1
B	540	HIS	-	EXPRESSION TAG	UNP A7Y7W1
B	541	HIS	-	EXPRESSION TAG	UNP A7Y7W1

- Molecule 2 is ALANINE (three-letter code: ALA) (formula: $C_3H_7NO_2$).



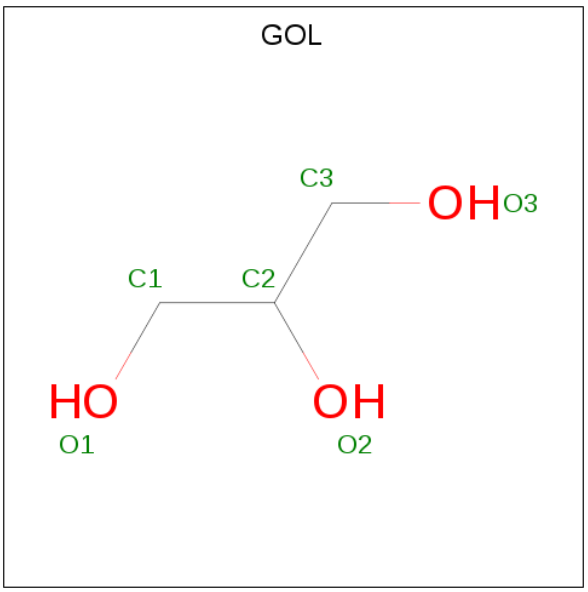
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 5 3 1 1	0	0
2	B	1	Total C N O 5 3 1 1	0	0

- Molecule 3 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 12 9 1 2	0	0
3	B	1	Total C N O 12 9 1 2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	349	Total O 349 349	0	0
5	B	337	Total O 337 337	0	0

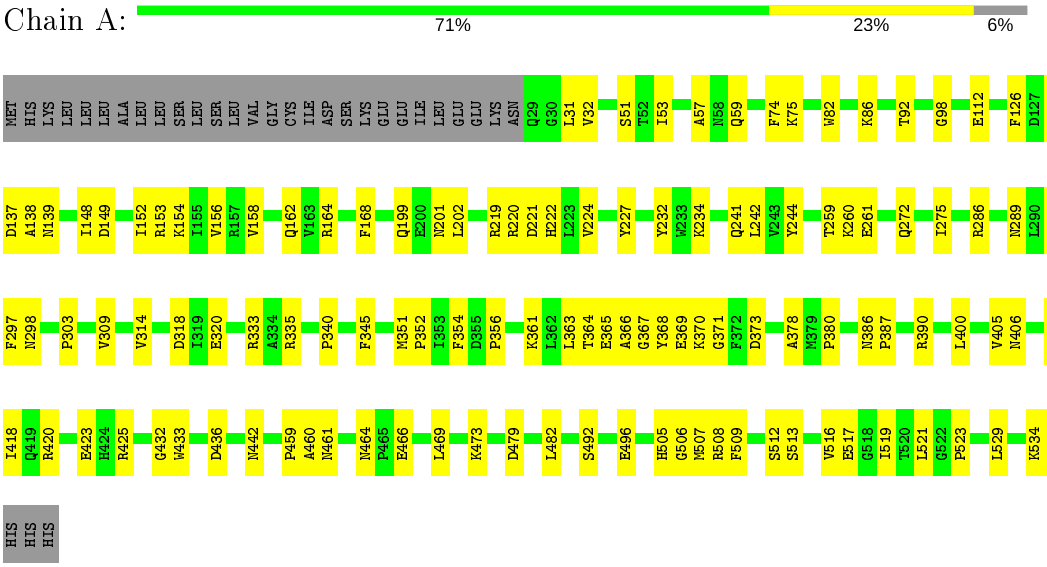
3 Residue-property plots (i)

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. 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. 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.

Note EDS failed to run properly.

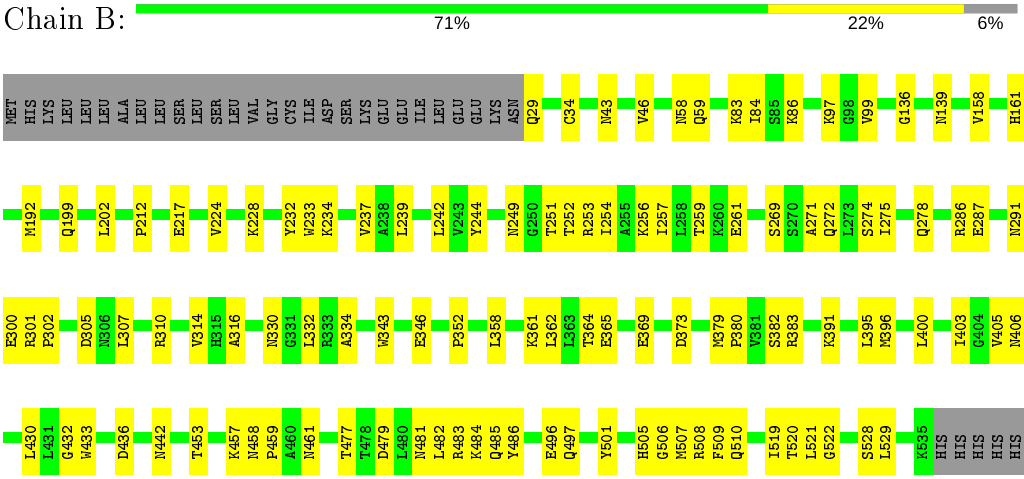
- Molecule 1: ABC transporter periplasmic peptide-binding protein

Chain A:



- Molecule 1: ABC transporter periplasmic peptide-binding protein

Chain B:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	106.14Å 106.14Å 100.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.99 – 1.75	Depositor
% Data completeness (in resolution range)	98.4 (33.99-1.75)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 1.75Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.160 , 0.184	Depositor
Wilson B-factor (Å^2)	23.1	Xtriage
Anisotropy	0.119	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	0.078 for -h,-k,l 0.320 for h,-h-k,-l 0.079 for -k,-h,-l	Xtriage
Total number of atoms	8932	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.38	1/4204 (0.0%)	0.55	1/5718 (0.0%)
1	B	0.36	0/4207	0.53	0/5722
All	All	0.37	1/8411 (0.0%)	0.54	1/11440 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	387	PRO	N-CD	5.55	1.55	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	386	ASN	C-N-CD	5.23	139.37	128.40

There are no chirality outliers.

There are no planarity outliers.

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	4098	0	4001	103	0
1	B	4102	0	4006	96	0
2	A	5	0	4	0	0
2	B	5	0	4	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	12	0	9	0	0
3	B	12	0	9	0	0
4	A	6	0	8	1	0
4	B	6	0	8	1	0
5	A	349	0	0	13	0
5	B	337	0	0	20	0
All	All	8932	0	8049	200	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 12.

All (200) 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:153:ARG:HH21	1:A:154:LYS:HE2	1.18	1.08
1:A:364:THR:HG22	1:A:369:GLU:HA	1.35	1.07
1:A:366:ALA:H	1:A:367:GLY:HA2	0.92	1.04
1:A:366:ALA:N	1:A:367:GLY:HA2	1.68	1.02
1:A:224:VAL:HG13	1:A:244:TYR:HB2	1.44	0.98
1:B:291:ASN:HD21	1:B:506:GLY:H	1.14	0.90
1:A:366:ALA:H	1:A:367:GLY:CA	1.83	0.89
1:B:287:GLU:OE2	1:B:521:LEU:HB3	1.72	0.89
1:A:291:ASN:HD21	1:A:506:GLY:H	1.23	0.85
1:A:425:ARG:HG3	5:A:1014:HOH:O	1.76	0.84
1:A:59:GLN:NE2	1:A:529:LEU:H	1.75	0.83
1:B:58:ASN:HA	5:B:847:HOH:O	1.80	0.81
1:A:314:VAL:HG11	1:A:352:PRO:HG2	1.63	0.80
1:B:299:THR:HB	5:B:967:HOH:O	1.80	0.80
1:B:496[A]:GLU:HG2	1:B:497:GLN:HG2	1.64	0.80
1:B:59:GLN:NE2	1:B:529:LEU:H	1.80	0.78
1:A:199:GLN:HB3	1:A:202:LEU:HD22	1.65	0.77
1:B:314[A]:VAL:HG11	1:B:352:PRO:HG2	1.68	0.76
1:B:242:LEU:HD11	1:B:529:LEU:HD12	1.68	0.75
1:A:294:TYR:CE2	1:A:432:GLY:HA2	2.22	0.74
1:A:98:GLY:HA2	1:A:112:GLU:OE1	1.89	0.72
1:B:269:SER:HB2	1:B:272:GLN:OE1	1.90	0.72
1:A:366:ALA:N	1:A:367:GLY:CA	2.45	0.71
1:A:479:ASP:HB3	1:A:482:LEU:HD12	1.73	0.70
1:A:361:LYS:O	1:A:361:LYS:HD3	1.92	0.69
1:B:346:GLU:HG2	5:B:825:HOH:O	1.90	0.69
1:B:224:VAL:HG13	1:B:244:TYR:HB2	1.72	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:SER:O	1:B:278:GLN:HG3	1.91	0.69
1:A:423:GLU:HB2	5:A:1014:HOH:O	1.92	0.69
1:A:364:THR:O	1:A:365:GLU:CB	2.41	0.67
1:A:298:ASN:HD21	1:A:461:ASN:HD22	1.41	0.66
1:A:153:ARG:NH2	1:A:154:LYS:HE2	2.02	0.65
1:A:436:ASP:H	1:A:442:ASN:ND2	1.93	0.65
1:B:310:ARG:NH1	5:B:967:HOH:O	2.30	0.65
1:B:86:LYS:HG2	5:B:783:HOH:O	1.96	0.65
1:A:436:ASP:H	1:A:442:ASN:HD21	1.45	0.64
1:B:234:LYS:HD2	5:B:993:HOH:O	1.96	0.64
1:B:477:THR:HG21	1:B:482:LEU:HD13	1.79	0.63
1:B:217:GLU:HB3	5:B:1025:HOH:O	1.98	0.63
1:B:314[A]:VAL:HG13	1:B:501:TYR:CE2	2.32	0.63
1:B:509:PHE:HD1	5:B:832:HOH:O	1.79	0.63
1:A:86:LYS:HD2	1:A:86:LYS:H	1.63	0.63
1:B:307:LEU:HB3	5:B:1021:HOH:O	1.99	0.62
1:B:436:ASP:H	1:B:442:ASN:HD21	1.47	0.62
1:B:332:LEU:HD12	4:B:603:GOL:H32	1.81	0.61
1:A:365:GLU:O	1:A:365:GLU:HG2	2.01	0.61
1:B:505:HIS:HE1	5:B:1033:HOH:O	1.81	0.61
1:B:287:GLU:OE2	1:B:521:LEU:CB	2.48	0.61
1:B:254:ILE:O	1:B:257:ILE:HG22	2.00	0.61
1:B:436:ASP:H	1:B:442:ASN:ND2	1.99	0.60
1:A:291:ASN:O	1:A:505:HIS:HD2	1.84	0.60
1:B:228:LYS:HB2	1:B:239:LEU:O	2.01	0.60
1:B:199:GLN:HB3	1:B:202:LEU:HD22	1.83	0.59
1:B:256:LYS:HA	1:B:259:THR:HG22	1.83	0.59
1:A:201:ASN:OD1	1:A:202:LEU:HD13	2.02	0.59
1:A:469:LEU:HG	1:A:473:LYS:HE3	1.85	0.59
1:B:97:LYS:HD3	1:B:161:HIS:NE2	2.18	0.59
1:A:519:ILE:H	1:A:519:ILE:HD13	1.67	0.58
1:B:232:TYR:CE2	1:B:234:LYS:HB3	2.38	0.58
1:B:364:THR:HG23	1:B:369:GLU:HB2	1.84	0.58
1:A:364:THR:O	1:A:365:GLU:HB3	2.03	0.56
1:A:512:SER:HB2	1:A:516:VAL:HG21	1.88	0.56
1:A:86:LYS:HD2	1:A:86:LYS:N	2.19	0.56
1:A:513:SER:O	1:A:516:VAL:HG22	2.06	0.56
1:A:139:ASN:ND2	5:A:917:HOH:O	2.38	0.56
1:B:519:ILE:O	5:B:963:HOH:O	2.18	0.56
1:A:363:LEU:O	1:A:366:ALA:HB3	2.06	0.55
1:B:259:THR:HG23	1:B:261:GLU:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:SER:O	1:A:496:GLU:HG2	2.06	0.55
1:A:320:GLU:HG2	1:A:333:ARG:NH1	2.22	0.55
1:B:380:PRO:HG3	1:B:412:TYR:O	2.06	0.54
1:B:136:GLY:HA3	5:B:814:HOH:O	2.09	0.53
1:A:519:ILE:N	1:A:519:ILE:HD13	2.24	0.53
1:A:365:GLU:H	1:A:367:GLY:HA2	1.74	0.53
1:A:479:ASP:CB	1:A:482:LEU:HD12	2.38	0.53
1:A:298:ASN:C	1:A:298:ASN:HD22	2.13	0.52
1:B:361:LYS:O	1:B:365:GLU:HG3	2.10	0.52
1:A:59:GLN:HE21	1:A:529:LEU:H	1.55	0.52
1:A:74:PHE:C	1:A:75:LYS:HD2	2.30	0.52
1:B:99:VAL:HG13	1:B:233:TRP:CD1	2.45	0.52
1:A:232:TYR:CE2	1:A:234:LYS:HB3	2.45	0.52
1:A:272:GLN:HA	1:A:275:ILE:HD13	1.92	0.51
1:B:391:LYS:HE3	1:B:395:LEU:HG	1.92	0.51
1:B:97:LYS:HD3	1:B:161:HIS:CD2	2.45	0.51
1:A:364:THR:HG22	1:A:369:GLU:CA	2.24	0.51
1:A:517:GLU:C	1:A:519:ILE:HD13	2.31	0.51
1:A:534:LYS:O	1:A:535:LYS:HB3	2.11	0.51
1:B:314[A]:VAL:HG13	1:B:501:TYR:CD2	2.46	0.51
1:A:509:PHE:HB2	5:A:846:HOH:O	2.12	0.50
1:A:505:HIS:HE1	5:A:1045:HOH:O	1.94	0.50
1:B:358:LEU:HD22	1:B:362:LEU:HG	1.94	0.50
1:B:302:PRO:HA	1:B:305:ASP:OD1	2.12	0.50
1:B:298:ASN:C	1:B:298:ASN:HD22	2.15	0.49
1:B:298:ASN:HD21	1:B:461:ASN:HD22	1.58	0.49
1:A:153:ARG:HG3	1:A:168:PHE:CE1	2.48	0.49
1:A:227[A]:TYR:CE1	1:A:241:GLN:HG2	2.47	0.49
1:B:84:ILE:HD11	1:B:175:LEU:HD11	1.95	0.49
1:A:464:ASN:OD1	1:A:466:GLU:HB2	2.13	0.49
1:A:74:PHE:O	1:A:75:LYS:HD2	2.12	0.49
1:B:287:GLU:OE2	1:B:522:GLY:N	2.45	0.49
1:A:158:VAL:HG21	1:A:162:GLN:OE1	2.12	0.49
1:A:400:LEU:HB3	1:A:405:VAL:HB	1.94	0.49
1:B:362:LEU:HB3	5:B:786:HOH:O	2.11	0.49
1:B:482:LEU:HD22	1:B:486:TYR:CE2	2.47	0.49
1:A:370:LYS:HA	1:A:370:LYS:HE3	1.95	0.48
1:B:330:ASN:HB2	5:B:846:HOH:O	2.12	0.48
1:B:433:TRP:HE1	1:B:442:ASN:ND2	2.10	0.48
1:A:335:ARG:HG3	5:A:1049:HOH:O	2.13	0.48
1:B:453:THR:HA	5:B:838:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:ILE:HA	5:B:917:HOH:O	2.13	0.48
1:A:420:ARG:HA	5:A:1014:HOH:O	2.14	0.48
1:B:286:ARG:O	1:B:286:ARG:HG2	2.14	0.48
1:A:242:LEU:HD21	1:A:529:LEU:HD13	1.96	0.47
1:B:34:CYS:HB3	1:B:253:ARG:HG2	1.96	0.47
1:B:286:ARG:HH11	1:B:286:ARG:HG3	1.79	0.47
1:A:156:VAL:HG21	1:A:164:ARG:HH21	1.78	0.47
1:B:259:THR:CG2	1:B:261:GLU:HG3	2.44	0.47
1:B:507:MET:HB2	1:B:509:PHE:CZ	2.50	0.47
1:B:271:ALA:HB3	1:B:272:GLN:NE2	2.30	0.47
1:A:222:HIS:HB2	5:A:911:HOH:O	2.14	0.47
1:B:249:ASN:HD22	1:B:252:THR:H	1.63	0.47
1:A:369:GLU:C	1:A:371:GLY:H	2.17	0.47
1:A:298:ASN:ND2	1:A:461:ASN:HD22	2.10	0.47
1:B:158:VAL:HG11	1:B:162:GLN:OE1	2.15	0.47
1:A:259:THR:OG1	1:A:261:GLU:HG3	2.15	0.46
1:A:380:PRO:HA	1:A:411:GLU:OE2	2.15	0.46
1:A:126:PHE:CE2	1:A:152:ILE:HG21	2.50	0.46
1:A:294:TYR:OH	1:A:459:PRO:HG2	2.16	0.46
1:A:318:ASP:HB3	5:A:748:HOH:O	2.13	0.46
1:B:294:TYR:CE2	1:B:432:GLY:HA2	2.51	0.46
1:B:520:THR:OG1	1:B:528:SER:HB3	2.16	0.46
1:B:287:GLU:HG2	1:B:508:ARG:HB3	1.98	0.46
1:B:287:GLU:CD	1:B:522:GLY:H	2.19	0.46
1:B:379:MET:HG2	1:B:414:TRP:HZ3	1.81	0.46
1:A:364:THR:HB	1:A:369:GLU:HG2	1.98	0.46
1:A:370:LYS:CA	1:A:370:LYS:HE3	2.46	0.46
1:A:148:ILE:CG2	1:A:149:ASP:N	2.79	0.45
1:B:294:TYR:OH	1:B:459:PRO:HG2	2.17	0.45
1:A:354:PHE:CE1	1:A:356:PRO:HG3	2.51	0.45
1:A:378:ALA:O	1:A:411:GLU:HG3	2.17	0.45
1:A:137:ASP:O	1:A:138:ALA:HB3	2.16	0.45
1:A:414:TRP:CH2	1:A:418:ILE:HD11	2.52	0.45
1:A:59:GLN:HE22	1:A:529:LEU:H	1.61	0.45
1:B:510:GLN:HB2	1:B:521:LEU:HD11	1.99	0.45
1:B:458:ASN:HA	1:B:459:PRO:HD3	1.79	0.45
1:B:291:ASN:O	1:B:505:HIS:HD2	1.99	0.45
1:A:508:ARG:HD3	1:A:521:LEU:HB3	1.99	0.45
1:A:219:ARG:HB2	1:A:222:HIS:HB3	2.00	0.44
1:A:31:LEU:HD23	1:A:32:VAL:N	2.32	0.44
1:B:298:ASN:HD22	1:B:300:GLU:H	1.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:ASN:ND2	1:B:252:THR:H	2.15	0.44
1:B:43:ASN:O	1:B:46:VAL:HG22	2.17	0.44
1:A:156:VAL:HG21	1:A:164:ARG:NH2	2.33	0.44
1:A:373:ASP:CG	1:A:406:ASN:HD22	2.20	0.44
1:B:358:LEU:CD2	1:B:362:LEU:HG	2.47	0.44
1:B:139:ASN:ND2	5:B:893:HOH:O	2.47	0.44
1:B:286:ARG:N	1:B:286:ARG:HD3	2.32	0.44
1:B:249:ASN:ND2	1:B:251:THR:H	2.15	0.44
1:B:316:ALA:HB2	1:B:403:ILE:HD13	1.99	0.44
1:B:212:PRO:O	1:B:237:VAL:HG21	2.17	0.44
1:B:479:ASP:O	1:B:483:ARG:HG3	2.18	0.44
1:B:301:ARG:HA	1:B:302:PRO:HD3	1.84	0.44
1:A:390:ARG:HG3	5:A:972:HOH:O	2.17	0.43
1:A:297:PHE:O	1:A:460:ALA:HA	2.18	0.43
1:A:260:LYS:HD2	5:A:977:HOH:O	2.17	0.43
1:A:340:PRO:HA	1:A:345:PHE:CG	2.53	0.43
1:B:249:ASN:C	1:B:249:ASN:HD22	2.22	0.43
1:B:29:GLN:HA	5:B:945:HOH:O	2.17	0.43
1:A:363:LEU:O	1:A:368:TYR:N	2.51	0.43
1:A:365:GLU:N	1:A:367:GLY:HA2	2.33	0.43
1:A:519:ILE:H	1:A:519:ILE:CD1	2.28	0.43
1:B:188:LYS:O	1:B:192:MET:HG2	2.18	0.43
1:B:400:LEU:HB3	1:B:405:VAL:HB	2.00	0.43
1:A:51:SER:HG	1:A:414:TRP:HE1	1.66	0.42
4:A:603:GOL:C1	5:A:799:HOH:O	2.67	0.42
1:B:275:ILE:HG13	5:B:959:HOH:O	2.19	0.42
1:A:138:ALA:HB1	5:A:843:HOH:O	2.19	0.42
1:B:481:ASN:O	1:B:485:GLN:HG3	2.20	0.42
1:A:286:ARG:HG2	1:A:507:MET:HE2	2.02	0.42
1:A:220:ARG:O	1:A:221:ASP:HB2	2.20	0.42
1:A:227[A]:TYR:CD1	1:A:241:GLN:HG2	2.54	0.42
1:A:433:TRP:HE1	1:A:442:ASN:ND2	2.18	0.42
1:A:351:MET:HA	1:A:352:PRO:HD3	1.91	0.41
1:B:382:SER:O	1:B:383:ARG:HD2	2.20	0.41
1:A:289:ASN:HA	1:A:523:PRO:HA	2.02	0.41
1:B:83:LYS:HE2	1:B:83:LYS:HB2	1.72	0.41
1:B:373:ASP:OD1	1:B:406:ASN:HB3	2.21	0.41
1:A:364:THR:O	1:A:365:GLU:HB2	2.20	0.41
1:B:457:LYS:HD2	1:B:457:LYS:HA	1.82	0.41
1:B:396:MET:SD	1:B:430:LEU:HD21	2.61	0.41
1:A:82:TRP:HA	1:A:92:THR:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ALA:HA	1:B:505:HIS:CE1	2.56	0.40
1:A:224:VAL:CG1	1:A:244:TYR:HB2	2.32	0.40
1:B:29:GLN:N	5:B:945:HOH:O	2.55	0.40
1:B:343:TRP:O	1:B:484:LYS:HD2	2.21	0.40
1:A:128:VAL:HA	1:A:133:HIS:CD2	2.56	0.40
1:A:303:PRO:HB2	1:A:309:VAL:HG21	2.03	0.40
1:B:400:LEU:HD12	1:B:407:VAL:HG21	2.02	0.40
1:A:365:GLU:H	1:A:367:GLY:CA	2.34	0.40
1:A:53:ILE:HG23	1:A:57:ALA:HB2	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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)

6 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	$\#\|Z\| > 2$
4	GOL	B	603	-	5,5,5	0.38	0	5,5,5	0.59	0
2	ALA	A	601	3	3,4,5	0.64	0	2,4,6	0.85	0
3	PHE	B	602	2	9,12,12	0.33	0	10,15,15	0.58	0
3	PHE	A	602	2	9,12,12	0.50	0	10,15,15	0.51	0
2	ALA	B	601	3	3,4,5	0.78	0	2,4,6	0.84	0
4	GOL	A	603	-	5,5,5	0.39	0	5,5,5	0.35	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
4	GOL	B	603	-	-	2/4/4/4	-
2	ALA	A	601	3	-	0/0/2/4	-
3	PHE	B	602	2	-	2/4/8/8	0/1/1/1
3	PHE	A	602	2	-	2/4/8/8	0/1/1/1
2	ALA	B	601	3	-	0/0/2/4	-
4	GOL	A	603	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	603	GOL	O1-C1-C2-C3
3	B	602	PHE	CA-CB-CG-CD1
3	B	602	PHE	CA-CB-CG-CD2

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Mol	Chain	Res	Type	Atoms
4	B	603	GOL	O1-C1-C2-O2
3	A	602	PHE	CA-CB-CG-CD1
3	A	602	PHE	CA-CB-CG-CD2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	603	GOL	1	0
4	A	603	GOL	1	0

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.