



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 03:08 pm GMT

PDB ID : 4QFP  
Title : Crystal structure of dipeptide binding protein from pseudoalteromonas sp. SM9913 in complex with Val-Thr  
Authors : Li, C.Y.; Zhang, Y.Z.  
Deposited on : 2014-05-21  
Resolution : 1.90 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

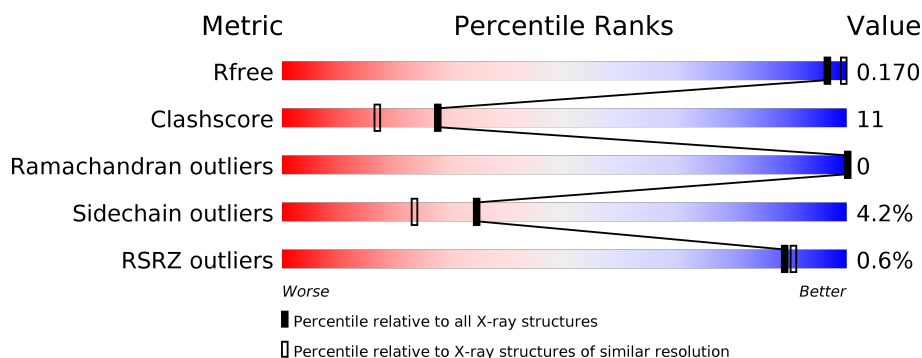
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	5047 (1.90-1.90)
Clashscore	112137	5731 (1.90-1.90)
Ramachandran outliers	110173	5669 (1.90-1.90)
Sidechain outliers	110143	5670 (1.90-1.90)
RSRZ outliers	101464	5100 (1.90-1.90)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	541	<div> <div></div> <div>74% 18% 6%</div> </div>
1	B	541	<div> <div></div> <div>73% 18% 6%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	VAL	B	601	-	-	-	X
3	THR	B	602	-	-	X	X
5	GOL	B	604	-	-	X	X
5	GOL	B	605	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9102 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.

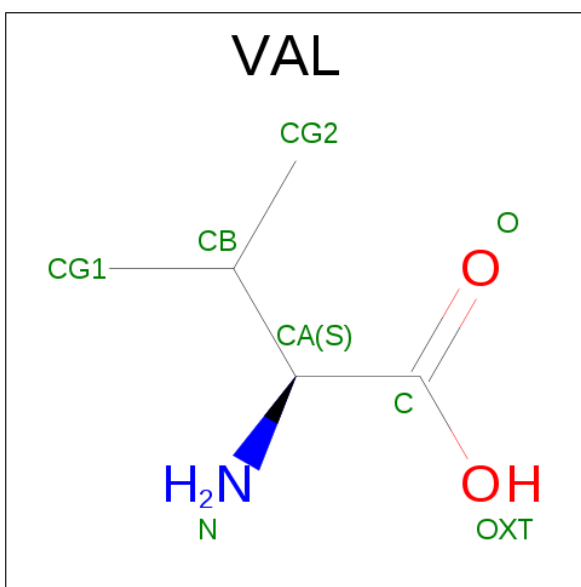
- Molecule 1 is a protein called ABC transporter periplasmic peptide-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	507	Total	C	N	O	S	0	9	0
			4146	2655	701	776	14			
1	B	507	Total	C	N	O	S	0	2	0
			4098	2628	691	765	14			

There are 12 discrepancies between the modelled and reference sequences:

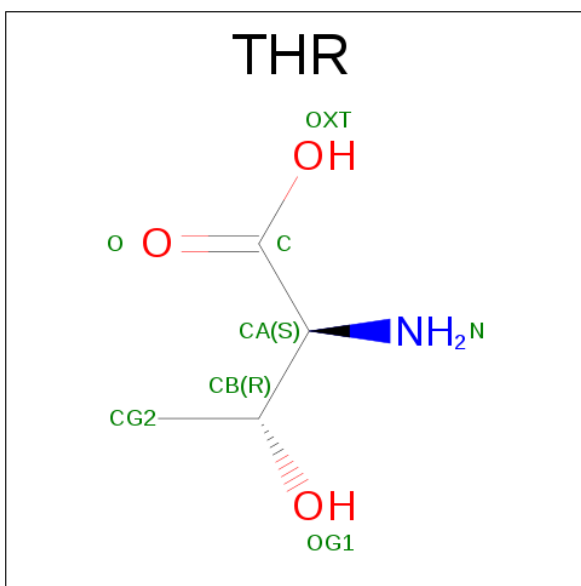
Chain	Residue	Modelled	Actual	Comment	Reference
A	536	HIS	-	EXPRESSION TAG	UNP A7Y7W1
A	537	HIS	-	EXPRESSION TAG	UNP A7Y7W1
A	538	HIS	-	EXPRESSION TAG	UNP A7Y7W1
A	539	HIS	-	EXPRESSION TAG	UNP A7Y7W1
A	540	HIS	-	EXPRESSION TAG	UNP A7Y7W1
A	541	HIS	-	EXPRESSION TAG	UNP A7Y7W1
B	536	HIS	-	EXPRESSION TAG	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 VALINE (three-letter code: VAL) (formula: C<sub>5</sub>H<sub>11</sub>NO<sub>2</sub>).



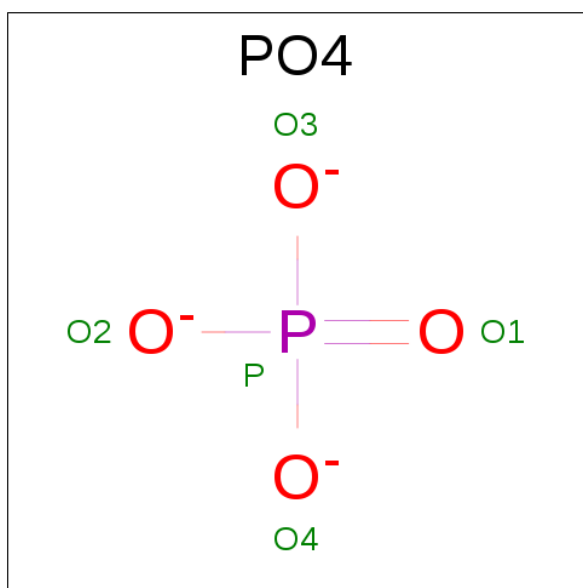
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			7	5	1	1		
2	B	1	Total	C	N	O	0	0
			7	5	1	1		

- Molecule 3 is THREONINE (three-letter code: THR) (formula: C<sub>4</sub>H<sub>9</sub>NO<sub>3</sub>).



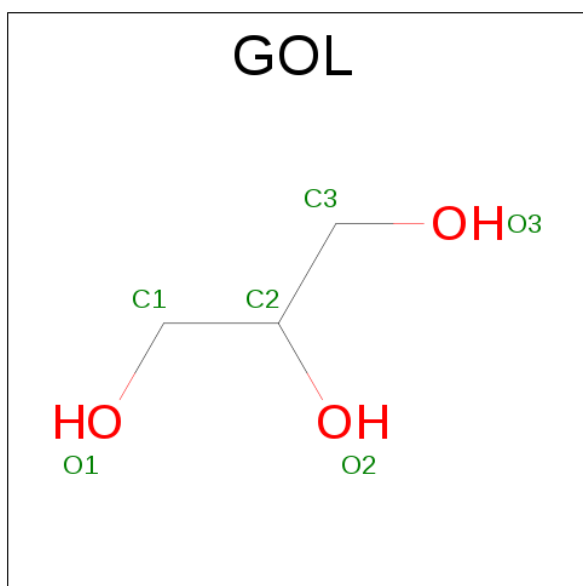
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			8	4	1	3		
3	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	385	Total	O	0	0
			385	385		
6	B	421	Total	O	0	0
			421	421		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.95Å 105.95Å 101.26Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.68 – 1.90 34.68 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (34.68-1.90) 99.2 (34.68-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 1.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.155 , 0.177 0.148 , 0.170	Depositor DCC
$R_{free}$ test set	4936 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.9	Xtriage
Anisotropy	0.208	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 32.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.070 for -h,-k,l 0.269 for h,-h-k,-l 0.074 for -k,-h,-l	Xtriage
Reported twinning fraction	0.279 for h,-h-k,-l	Depositor
Outliers	0 of 98918 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	9102	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4

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	0.32	0/4252	0.51	0/5782
1	B	0.34	1/4204 (0.0%)	0.51	1/5718 (0.0%)
All	All	0.33	1/8456 (0.0%)	0.51	1/11500 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	387	PRO	N-CD	5.43	1.55	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	386	ASN	C-N-CD	5.29	139.51	128.40

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	4146	0	4045	86	0
1	B	4098	0	4001	100	0
2	A	7	0	8	0	0
2	B	7	0	8	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	8	0	7	0	0
3	B	8	0	7	9	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	B	12	0	16	8	0
6	A	385	0	0	6	0
6	B	421	0	0	15	0
All	All	9102	0	8092	186	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 11.

All (186) 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:383:ARG:HH21	3:B:602:THR:HG21	1.12	1.10
1:B:50:GLY:H	3:B:602:THR:HG22	1.27	0.99
1:B:38:ASN:HD21	1:B:221:ASP:H	1.16	0.93
1:A:291:ASN:HD21	1:A:506:GLY:H	1.13	0.91
1:B:383:ARG:NH2	3:B:602:THR:HG21	1.86	0.89
1:A:38:ASN:HD21	1:A:221:ASP:H	1.15	0.89
1:A:86:LYS:H	1:A:86:LYS:HD2	1.35	0.89
1:B:272:GLN:HA	1:B:275:ILE:HD13	1.56	0.87
1:B:50:GLY:N	3:B:602:THR:HG22	1.90	0.87
1:B:366:ALA:H	1:B:367:GLY:HA2	1.40	0.85
1:B:291:ASN:HD21	1:B:506:GLY:H	1.22	0.83
1:A:349[A]:LYS:H	1:A:349[A]:LYS:HE2	1.47	0.80
1:B:275:ILE:HD12	1:B:275:ILE:H	1.46	0.78
1:A:249:ASN:HD21	1:A:251:THR:HB	1.48	0.78
1:A:492:SER:O	1:A:496[B]:GLU:HG3	1.83	0.77
1:B:38:ASN:ND2	1:B:221:ASP:H	1.83	0.76
1:A:86:LYS:CD	1:A:86:LYS:H	1.97	0.76
1:B:368:TYR:HE1	6:B:975:HOH:O	1.68	0.75
1:A:286:ARG:HB2	1:A:507:MET:HE3	1.70	0.74
1:A:59:GLN:NE2	1:A:529:LEU:H	1.87	0.72
1:B:50:GLY:CA	3:B:602:THR:HG22	2.20	0.71
1:A:38:ASN:ND2	1:A:221:ASP:H	1.89	0.71
1:A:199:GLN:HB3	1:A:202:LEU:HD22	1.71	0.70
1:B:149:ASP:HB3	6:B:1120:HOH:O	1.92	0.69
1:B:275:ILE:HD12	1:B:275:ILE:N	2.07	0.69
1:A:534:LYS:O	1:A:535:LYS:HB3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:GLY:HA3	3:B:602:THR:HG22	1.76	0.68
1:B:158:VAL:HG22	1:B:162:GLN:HB3	1.76	0.67
1:B:519:ILE:HG23	6:B:949:HOH:O	1.94	0.67
1:A:436:ASP:H	1:A:442:ASN:ND2	1.93	0.66
1:A:535:LYS:HG3	6:A:808:HOH:O	1.96	0.65
1:B:59:GLN:NE2	1:B:529:LEU:H	1.95	0.65
1:A:380:PRO:HG3	1:A:412:TYR:O	1.97	0.65
1:B:110:THR:HB	1:B:189:GLU:OE2	1.97	0.64
1:B:275:ILE:H	1:B:275:ILE:CD1	2.10	0.64
1:B:286:ARG:HG2	1:B:507:MET:HE2	1.78	0.64
1:A:38:ASN:HD21	1:A:221:ASP:N	1.93	0.64
1:B:153:ARG:HG3	1:B:168:PHE:CZ	2.33	0.64
1:B:98:GLY:HA2	1:B:112:GLU:OE1	1.98	0.63
1:B:123:SER:HA	1:B:126:PHE:CE2	2.33	0.63
1:A:361:LYS:O	1:A:365:GLU:HG3	1.96	0.63
1:A:249:ASN:C	1:A:249:ASN:HD22	2.02	0.62
1:B:366:ALA:N	1:B:367:GLY:HA2	2.06	0.62
1:B:510:GLN:HB2	5:B:604:GOL:H31	1.80	0.62
1:B:508:ARG:HD3	1:B:521:LEU:HB3	1.82	0.61
1:B:383:ARG:HH21	3:B:602:THR:CG2	2.00	0.61
1:A:287:GLU:HG3	1:A:521:LEU:O	2.00	0.61
1:B:510:GLN:HB2	5:B:604:GOL:C3	2.31	0.61
1:A:436:ASP:H	1:A:442:ASN:HD21	1.48	0.60
1:B:50:GLY:H	3:B:602:THR:CG2	2.11	0.60
1:A:294:TYR:CE2	1:A:432:GLY:HA2	2.38	0.59
1:A:228:LYS:HB3	1:A:239:LEU:O	2.02	0.59
1:B:527:ILE:HD11	5:B:604:GOL:H2	1.84	0.59
1:A:124:ARG:O	1:A:124:ARG:HG3	2.02	0.59
1:B:225:ARG:HD3	6:B:948:HOH:O	2.01	0.59
1:B:81:ASP:OD2	1:B:83:LYS:HE2	2.03	0.59
1:B:298:ASN:HD21	1:B:461:ASN:HD22	1.48	0.59
1:A:124:ARG:HD2	1:A:140:TYR:OH	2.03	0.59
1:B:335:ARG:HG3	6:B:788:HOH:O	2.03	0.58
1:B:224:VAL:HG13	1:B:244:TYR:HB2	1.86	0.58
1:A:286:ARG:HG3	1:A:507:MET:HE1	1.84	0.58
1:B:366:ALA:H	1:B:367:GLY:CA	2.13	0.57
1:B:509:PHE:O	5:B:604:GOL:H31	2.04	0.57
1:B:153:ARG:HG3	1:B:168:PHE:CE1	2.39	0.57
1:A:513:SER:O	1:A:516[A]:VAL:HG22	2.03	0.57
1:A:358:LEU:HD22	1:A:362:LEU:HG	1.85	0.57
1:B:365:GLU:HG3	1:B:365:GLU:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:LEU:O	1:B:366:ALA:HB3	2.05	0.56
1:B:496:GLU:HG3	6:B:1082:HOH:O	2.05	0.56
1:B:380:PRO:HG3	1:B:412:TYR:O	2.05	0.56
1:A:349[A]:LYS:H	1:A:349[A]:LYS:CE	2.15	0.56
1:B:348:GLN:HG3	1:B:495:ILE:HG13	1.87	0.56
1:A:493:MET:HA	1:A:496[A]:GLU:HG2	1.88	0.56
1:A:158[A]:VAL:HG21	1:A:162:GLN:OE1	2.05	0.56
1:B:298:ASN:C	1:B:298:ASN:HD22	2.09	0.55
1:A:291:ASN:O	1:A:505:HIS:HD2	1.90	0.55
1:B:406:ASN:HB2	6:B:991:HOH:O	2.07	0.54
1:A:390:ARG:C	1:A:390:ARG:HD3	2.27	0.54
1:B:434:ALA:N	2:B:601:VAL:O	2.36	0.53
1:B:291:ASN:O	1:B:505:HIS:HD2	1.92	0.53
1:B:534:LYS:O	1:B:535:LYS:HB3	2.09	0.53
1:B:68:ASP:OD1	1:B:70:VAL:HG13	2.09	0.53
1:B:231:ASP:HB2	6:B:1013:HOH:O	2.09	0.52
1:A:390:ARG:HD2	1:A:394:GLU:OE2	2.08	0.52
1:B:455:SER:HB3	6:B:947:HOH:O	2.09	0.52
1:A:353:ILE:HD12	1:A:354:PHE:H	1.74	0.52
1:A:361:LYS:HE2	1:A:365:GLU:OE2	2.09	0.52
1:B:151:LEU:HG	1:B:167:LEU:HD22	1.92	0.51
1:B:67:ILE:HD13	1:B:438:PRO:HD2	1.92	0.51
1:A:97:LYS:HD3	1:A:161:HIS:NE2	2.26	0.51
1:B:436:ASP:H	1:B:442:ASN:ND2	2.09	0.50
1:A:512:SER:HB2	1:A:516[A]:VAL:HG21	1.93	0.50
1:B:132:TYR:HA	1:B:135:VAL:HG23	1.92	0.50
1:A:223:LEU:HD12	1:A:223:LEU:C	2.31	0.50
1:A:348:GLN:HA	1:A:349[A]:LYS:HE2	1.92	0.50
1:B:153:ARG:NH2	1:B:154:LYS:HE2	2.26	0.50
1:B:370:LYS:HB2	1:B:370:LYS:HZ2	1.77	0.50
1:A:437:THR:HB	1:A:438:PRO:HD2	1.94	0.49
1:A:390:ARG:O	1:A:390:ARG:HD3	2.11	0.49
1:B:363:LEU:O	1:B:368:TYR:N	2.38	0.49
1:B:115:ALA:HB1	1:B:163:VAL:CG1	2.43	0.49
1:B:267:HIS:CE1	5:B:604:GOL:H11	2.47	0.49
1:B:366:ALA:N	1:B:367:GLY:CA	2.73	0.49
1:B:99:VAL:HB	1:B:113:PHE:HB3	1.95	0.48
1:A:433:TRP:HE1	1:A:442:ASN:ND2	2.11	0.48
1:A:505:HIS:HE1	6:A:1084:HOH:O	1.96	0.48
1:A:219:ARG:NH2	1:A:222:HIS:ND1	2.62	0.48
1:B:220:ARG:O	1:B:221:ASP:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:LYS:HD2	1:A:86:LYS:N	2.16	0.48
1:B:48:THR:O	2:B:601:VAL:HA	2.14	0.47
1:A:325:ALA:O	1:A:391:LYS:HE3	2.14	0.47
1:B:333:ARG:HH22	1:B:353:ILE:HD12	1.79	0.47
1:A:265:THR:CG2	1:A:511:ALA:HB3	2.45	0.47
1:A:86:LYS:CD	1:A:86:LYS:N	2.73	0.47
1:B:227[A]:TYR:CE1	1:B:241:GLN:HG2	2.50	0.47
1:A:363:LEU:HD23	1:A:363:LEU:HA	1.75	0.46
1:A:223:LEU:O	1:A:223:LEU:HD12	2.14	0.46
1:A:286:ARG:HB2	1:A:507:MET:CE	2.42	0.46
1:A:249:ASN:ND2	1:A:251:THR:H	2.13	0.46
1:A:161:HIS:HE1	6:A:854:HOH:O	1.98	0.46
1:A:219:ARG:HH21	1:A:222:HIS:CE1	2.34	0.46
1:A:249:ASN:ND2	1:A:249:ASN:C	2.69	0.46
1:B:288:THR:OG1	5:B:605:GOL:H2	2.16	0.46
1:B:382:SER:O	1:B:383:ARG:HD2	2.16	0.45
1:B:80:THR:HG21	6:B:711:HOH:O	2.16	0.45
1:A:232:TYR:CE2	1:A:234:LYS:HB3	2.52	0.45
1:A:249:ASN:ND2	1:A:252:THR:H	2.14	0.45
1:B:288:THR:HG22	6:B:763:HOH:O	2.17	0.45
1:B:149:ASP:OD1	1:B:150:GLN:N	2.48	0.45
1:A:378:ALA:O	1:A:411:GLU:HG2	2.17	0.45
1:A:447:LEU:HD11	6:A:790:HOH:O	2.17	0.45
1:B:436:ASP:HB3	6:B:772:HOH:O	2.17	0.45
1:B:82:TRP:C	1:B:83:LYS:HD2	2.37	0.45
1:A:479:ASP:O	1:A:483:ARG:HG3	2.17	0.44
1:A:59:GLN:HE22	1:A:529:LEU:H	1.64	0.44
1:B:535:LYS:C	1:B:535:LYS:HE2	2.38	0.44
1:A:320:GLU:HA	1:A:320:GLU:OE1	2.18	0.44
1:A:84:ILE:HG12	1:A:91:VAL:HG22	1.99	0.44
1:B:364:THR:C	1:B:366:ALA:H	2.21	0.44
1:B:50:GLY:HA3	3:B:602:THR:CG2	2.46	0.44
1:A:496[A]:GLU:HG3	1:A:497:GLN:HG2	1.99	0.44
1:A:265:THR:HG22	1:A:511:ALA:HB3	1.99	0.44
1:B:433:TRP:HE1	1:B:442:ASN:ND2	2.16	0.44
1:A:382[B]:SER:O	1:A:383:ARG:HD2	2.17	0.43
1:B:298:ASN:HD22	1:B:300:GLU:H	1.65	0.43
1:B:340:PRO:HA	1:B:345:PHE:CG	2.53	0.43
1:B:379:MET:HG3	1:B:379:MET:H	1.48	0.43
1:A:286:ARG:HA	1:A:508:ARG:O	2.18	0.43
1:A:249:ASN:ND2	1:A:251:THR:N	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:TYR:CZ	1:A:194:LEU:HD11	2.54	0.42
1:B:227[A]:TYR:CD1	1:B:241:GLN:HG2	2.54	0.42
1:B:505:HIS:CE1	6:B:1114:HOH:O	2.72	0.42
1:B:509:PHE:O	5:B:604:GOL:C3	2.67	0.42
1:B:228:LYS:HB2	1:B:239:LEU:O	2.18	0.42
1:B:340:PRO:HA	1:B:345:PHE:CD2	2.54	0.42
1:B:135:VAL:CG1	1:B:136:GLY:N	2.83	0.42
1:B:510:GLN:HB2	5:B:604:GOL:H32	2.02	0.42
1:A:308:LYS:HD3	6:A:798:HOH:O	2.19	0.41
1:A:423:GLU:OE1	1:A:425:ARG:NE	2.49	0.41
1:A:82:TRP:HA	1:A:92:THR:O	2.20	0.41
1:B:222:HIS:CD2	6:B:837:HOH:O	2.73	0.41
1:A:308:LYS:HB3	1:A:366:ALA:HB2	2.03	0.41
1:B:68:ASP:HB2	1:B:75:LYS:HD3	2.01	0.41
1:A:348:GLN:HG3	1:A:495:ILE:HG13	2.02	0.41
1:B:291:ASN:HD22	1:B:385:TYR:HB3	1.86	0.41
1:B:380:PRO:HA	1:B:411:GLU:OE2	2.20	0.41
1:B:199:GLN:HB3	1:B:202:LEU:HD22	2.03	0.41
1:B:414:TRP:CH2	1:B:418:ILE:HD11	2.56	0.41
1:A:271:ALA:HB2	1:A:328:TYR:CE2	2.56	0.41
1:B:363:LEU:HD23	1:B:363:LEU:HA	1.80	0.41
1:A:349[A]:LYS:H	1:A:349[A]:LYS:CD	2.33	0.41
1:A:119:ILE:CD1	1:A:157:ARG:HB2	2.51	0.41
1:A:373:ASP:OD1	1:A:406:ASN:HB3	2.21	0.41
1:A:445:SER:HB2	1:A:446:PRO:HD3	2.02	0.41
1:B:149:ASP:OD1	1:B:149:ASP:C	2.59	0.41
1:B:333:ARG:NH2	6:B:1006:HOH:O	2.54	0.41
1:A:439:ASP:HA	1:A:440:PRO:HD3	1.93	0.40
1:B:330:ASN:O	1:B:507:MET:HG2	2.21	0.40
1:A:153:ARG:HG3	1:A:168:PHE:CE1	2.56	0.40
1:A:86:LYS:HD2	6:A:998:HOH:O	2.20	0.40
1:B:519:ILE:HD11	1:B:529:LEU:HD22	2.03	0.40
1:A:424[A]:HIS:CD2	1:A:461:ASN:ND2	2.88	0.40
1:B:358:LEU:O	1:B:362:LEU:HG	2.21	0.40
1:A:228:LYS:HE3	1:A:228:LYS:HB2	1.93	0.40
1:A:272:GLN:HG3	1:A:275:ILE:HD12	2.03	0.40
1:A:297:PHE:O	1:A:460:ALA:HA	2.22	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	514/541 (95%)	500 (97%)	14 (3%)	0	100	100
1	B	507/541 (94%)	488 (96%)	19 (4%)	0	100	100
All	All	1021/1082 (94%)	988 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	449/472 (95%)	429 (96%)	20 (4%)	32	21
1	B	442/472 (94%)	423 (96%)	19 (4%)	33	22
All	All	891/944 (94%)	852 (96%)	39 (4%)	34	22

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	LYS
1	A	110	THR
1	A	124	ARG
1	A	158[A]	VAL
1	A	158[B]	VAL
1	A	160	ASP
1	A	202	LEU
1	A	242	LEU

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Mol	Chain	Res	Type
1	A	249	ASN
1	A	285	GLU
1	A	298	ASN
1	A	332	LEU
1	A	349[A]	LYS
1	A	349[B]	LYS
1	A	358	LEU
1	A	363	LEU
1	A	390	ARG
1	A	461	ASN
1	A	513	SER
1	A	521	LEU
1	B	29	GLN
1	B	34	CYS
1	B	38	ASN
1	B	70	VAL
1	B	110	THR
1	B	139	ASN
1	B	149	ASP
1	B	158	VAL
1	B	224	VAL
1	B	242	LEU
1	B	265	THR
1	B	298	ASN
1	B	335	ARG
1	B	358	LEU
1	B	363	LEU
1	B	370	LYS
1	B	390	ARG
1	B	447	LEU
1	B	535	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	59	GLN
1	A	249	ASN
1	A	291	ASN
1	A	298	ASN
1	A	311	GLN
1	A	348	GLN

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Mol	Chain	Res	Type
1	A	442	ASN
1	A	461	ASN
1	A	497	GLN
1	A	505	HIS
1	B	38	ASN
1	B	58	ASN
1	B	59	GLN
1	B	291	ASN
1	B	298	ASN
1	B	311	GLN
1	B	348	GLN
1	B	350	ASN
1	B	357	GLN
1	B	442	ASN
1	B	485	GLN
1	B	497	GLN
1	B	505	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

8 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
2	VAL	A	601	3	6,6,7	0.83	0	6,7,9	2.09	1 (16%)
3	THR	A	602	2	4,7,7	0.51	0	3,9,9	0.39	0
4	PO4	A	603	-	4,4,4	0.73	0	6,6,6	0.49	0
2	VAL	B	601	3	6,6,7	1.50	1 (16%)	6,7,9	1.46	1 (16%)
3	THR	B	602	2	4,7,7	1.27	0	3,9,9	0.73	0
4	PO4	B	603	-	4,4,4	0.69	0	6,6,6	0.39	0
5	GOL	B	604	-	5,5,5	0.45	0	5,5,5	0.77	0
5	GOL	B	605	-	5,5,5	0.31	0	5,5,5	0.37	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
2	VAL	A	601	3	-	0/5/6/8	0/0/0/0
3	THR	A	602	2	-	0/4/8/8	0/0/0/0
4	PO4	A	603	-	-	0/0/0/0	0/0/0/0
2	VAL	B	601	3	-	0/5/6/8	0/0/0/0
3	THR	B	602	2	-	0/4/8/8	0/0/0/0
4	PO4	B	603	-	-	0/0/0/0	0/0/0/0
5	GOL	B	604	-	-	0/4/4/4	0/0/0/0
5	GOL	B	605	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	VAL	CA-C	3.58	1.55	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	VAL	CB-CA-C	-4.76	106.44	112.96
2	B	601	VAL	O-C-CA	-3.00	118.16	125.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	VAL	2	0
3	B	602	THR	9	0
5	B	604	GOL	7	0
5	B	605	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	507/541 (93%)	-0.21	5 (0%)	82 84	14, 22, 33, 42	0
1	B	507/541 (93%)	-0.20	1 (0%)	94 95	13, 22, 35, 49	0
All	All	1014/1082 (93%)	-0.20	6 (0%)	89 90	13, 22, 33, 49	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	424[A]	HIS	4.0
1	A	137	ASP	3.3
1	A	520	THR	2.6
1	A	357	GLN	2.2
1	A	227	TYR	2.2
1	B	520	THR	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	THR	B	602	8/8	0.87	0.15	8.41	18,21,25,26	0
5	GOL	B	605	6/6	0.90	0.21	5.22	20,22,27,32	0
2	VAL	B	601	7/8	0.92	0.12	4.64	15,16,17,18	0
5	GOL	B	604	6/6	0.90	0.16	2.93	17,19,20,24	0
2	VAL	A	601	7/8	0.97	0.09	1.18	13,14,17,18	0
4	PO4	A	603	5/5	0.98	0.09	-1.07	26,28,31,32	0
3	THR	A	602	8/8	0.97	0.06	-2.13	16,16,18,19	0
4	PO4	B	603	5/5	0.90	0.23	-	35,36,45,45	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.