Full wwPDB X-ray Structure Validation Report ⓘ

Apr 3, 2024 – 03:10 am BST

PDB ID	:	7NSN
Title	:	Multi-domain GH92 alpha-1,2-mannosidase from Neobacillus novalis: mannoimidazole complex
Authors	:	Kolaczkowski, B.M.; Moroz, O.V.; Blagova, E.; Davies, G.J.; Wilson, K.S.; Moeler, M.S.; Meyer, A.S.; Westh, P.; Jensen, K.; Krogh, K.B.R.M.
Deposited on	:	2021-03-08
Resolution	:	2.29 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

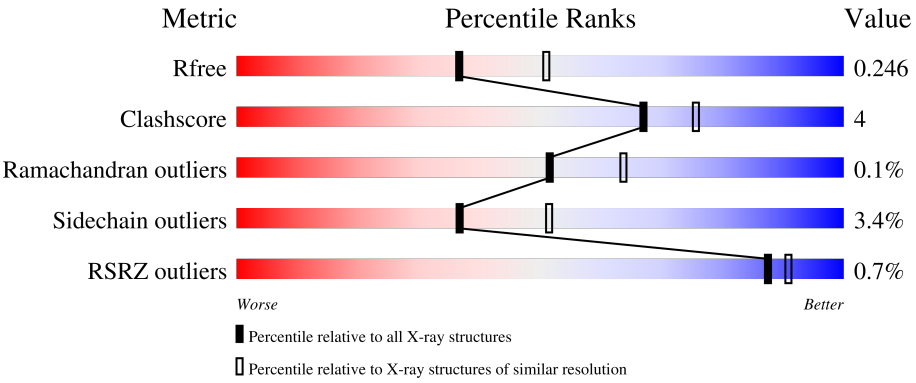
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.29 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	1411	87% 9%
1	B	1411	% 78% 8% 13%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 20790 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.

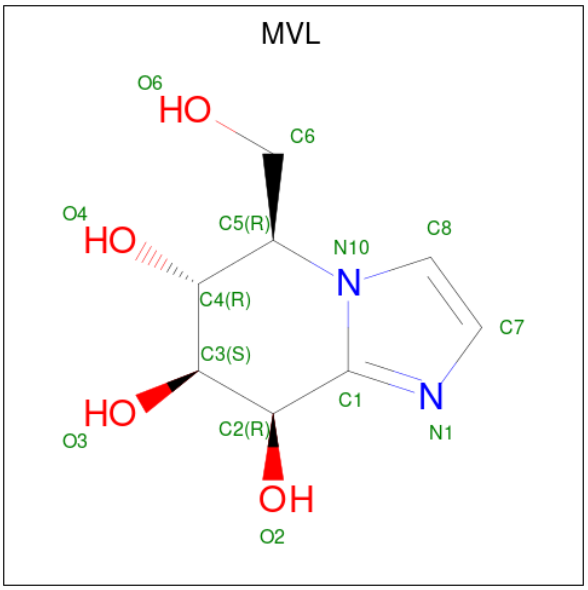
- Molecule 1 is a protein called GH92 alpha-1,2-mannosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1371	Total	C	N	O	S	0	0	0
			10648	6716	1789	2118	25			
1	B	1224	Total	C	N	O	S	0	0	0
			9492	5987	1597	1884	24			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

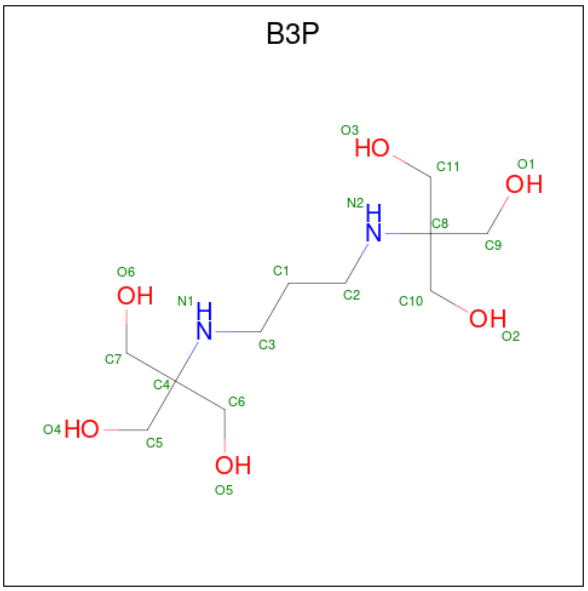
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Ca	0	0
			5	5		
2	B	4	Total	Ca	0	0
			4	4		

- Molecule 3 is (5R,6R,7S,8R)-5-(HYDROXYMETHYL)-5,6,7,8-TETRAHYDROIMIDAZO[1,2-A]PYRIDINE-6,7,8-TRIOL (three-letter code: MVL) (formula: $C_8H_{12}N_2O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 14 8 2 4	0	0
3	A	1	Total C N O 14 8 2 4	0	0
3	B	1	Total C N O 14 8 2 4	0	0

- Molecule 4 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula: $C_{11}H_{26}N_2O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 19 11 2 6	0	0
4	B	1	Total C N O 19 11 2 6	0	0

- Molecule 5 is water.

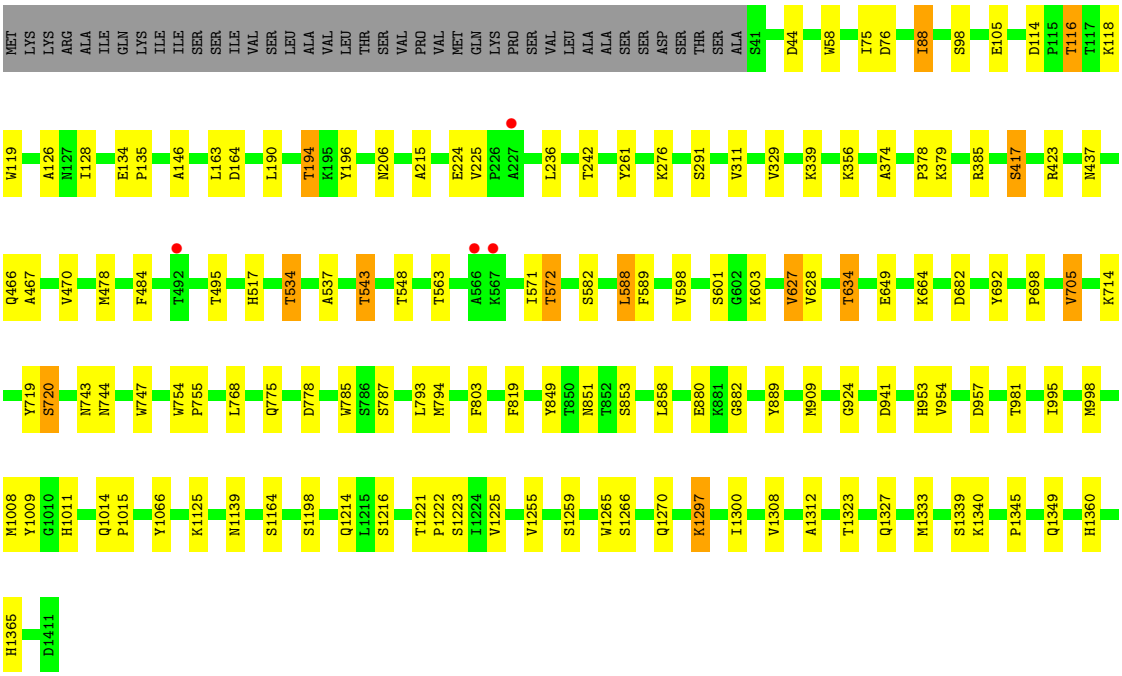
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	318	Total O 318 318	0	0
5	B	243	Total O 243 243	0	0

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 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.

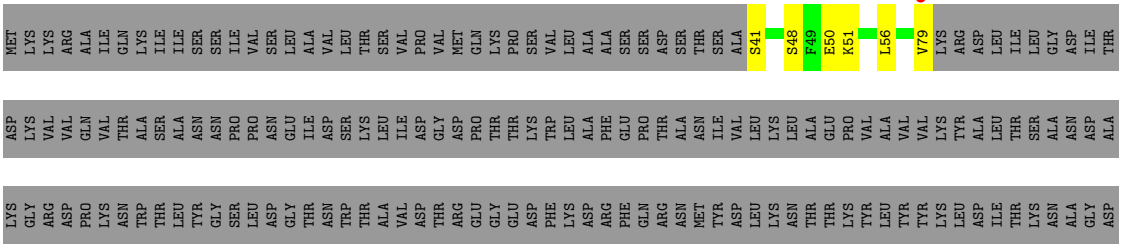
• Molecule 1: GH92 alpha-1,2-mannosidase

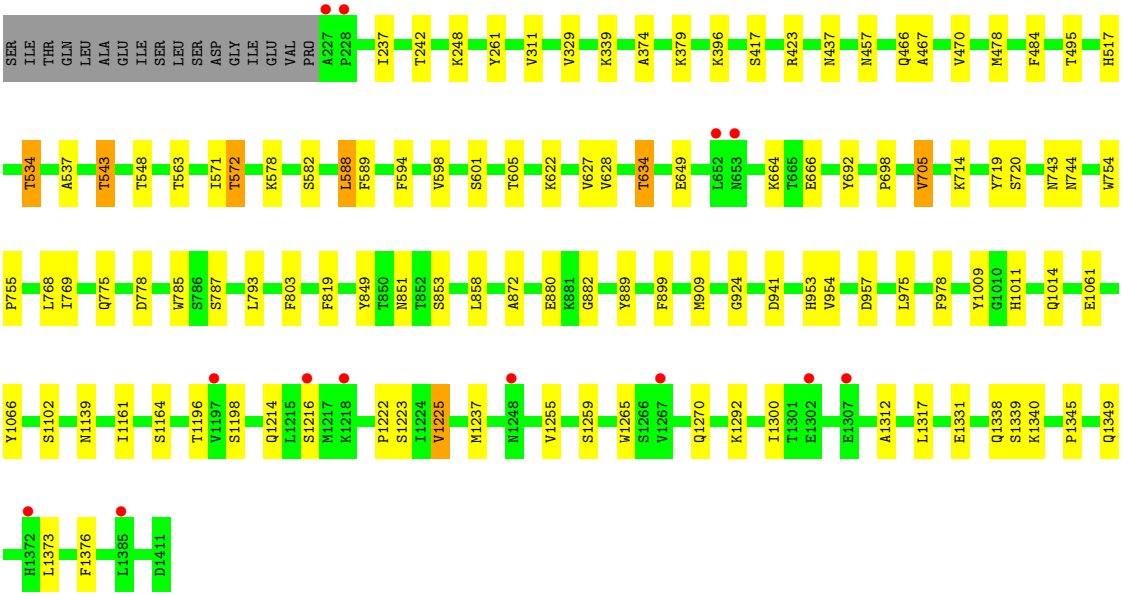
Chain A:



• Molecule 1: GH92 alpha-1,2-mannosidase

Chain B:




SER ILE THR GLN LEU ALA GLU ILE SER LEU SER ASP GLY ILE GLU VAL PRO A227 P228 I237 T242 K248 Y261 V311 V329 K339 A374 K379 K396 S417 R423 N437 M457 Q466 A467 V470 M478 F484 T495 H517
T534 A537 T543 T548 T563 I571 T572 K578 S582 L588 F589 F594 V598 S601 T605 K622 V627 V628 T634 E649 L652 M653 K664 T665 E666 Y692 P698 V706 K714 Y719 S720 N743 N744 W754
P755 L768 I769 Q775 D778 W785 S786 S787 L793 F803 F819 Y849 T850 N851 T852 S853 L858 A872 E880 K881 G882 Y889 F899 M909 G924 D941 H953 V954 D957 L975 F978 Y1009 G1010 H1011 Q1014 E1061
Y1066 S1102 N1139 I1161 S1164 T1196 V1197 S1198 Q1214 L1215 S1216 M1217 K1218 P1222 S1223 I1224 V1225 M1237 N1248 V1255 S1259 W1265 S1266 V1267 Q1270 K1292 I1300 T1301 E1302 E1307 A1312 L1317 E1331 Q1338 S1339 K1340 P1345 Q1349
H1372 L1373 F1376 L1385 D1411

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.61Å 151.94Å 114.01Å 90.00° 94.63° 90.00°	Depositor
Resolution (Å)	47.92 – 2.29 47.92 – 2.29	Depositor EDS
% Data completeness (in resolution range)	98.0 (47.92-2.29) 98.0 (47.92-2.29)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.205 , 0.246 0.205 , 0.246	Depositor DCC
R_{free} test set	6947 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	28.4	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 27.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20790	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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: B3P, CA, MVL

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	0.46	0/10900	0.80	0/14803
1	B	0.45	0/9721	0.79	0/13195
All	All	0.46	0/20621	0.80	0/27998

There are no bond length outliers.

There are no bond angle outliers.

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	10648	0	10216	84	0
1	B	9492	0	9068	67	0
2	A	5	0	0	0	0
2	B	4	0	0	0	0
3	A	28	0	22	2	0
3	B	14	0	10	3	0
4	A	19	0	26	1	0
4	B	19	0	26	1	0
5	A	318	0	0	6	0
5	B	243	0	0	7	0
All	All	20790	0	19368	153	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 4.

All (153) 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:995:ILE:HG12	1:A:998:MET:CE	1.71	1.19
1:A:995:ILE:HG12	1:A:998:MET:HE2	1.27	1.15
1:A:995:ILE:H	1:A:998:MET:HE3	1.11	1.14
1:B:534:THR:HG22	1:B:537:ALA:H	1.20	1.05
1:A:995:ILE:H	1:A:998:MET:CE	1.71	1.04
1:A:534:THR:HG22	1:A:537:ALA:H	1.17	1.03
1:A:417:SER:HB2	1:A:423:ARG:H	1.22	1.03
1:A:1333:MET:HE2	5:A:1646:HOH:O	1.60	1.00
1:B:478:MET:HE1	1:B:793:LEU:HD22	1.45	0.96
1:B:437:ASN:OD1	1:B:634:THR:HG21	1.70	0.90
1:A:385:ARG:HD2	5:A:1880:HOH:O	1.70	0.90
1:A:437:ASN:OD1	1:A:634:THR:HG21	1.71	0.90
1:A:995:ILE:N	1:A:998:MET:HE3	1.91	0.84
1:A:478:MET:HE1	1:A:793:LEU:HD22	1.59	0.83
1:A:995:ILE:HG12	1:A:998:MET:HE3	1.62	0.81
1:A:682:ASP:HB3	5:A:1913:HOH:O	1.81	0.80
1:B:478:MET:CE	1:B:793:LEU:HD22	2.14	0.77
1:B:478:MET:HE3	3:B:1505:MVL:H6C2	1.66	0.77
1:A:478:MET:HE3	3:A:1505:MVL:H6C2	1.68	0.75
1:A:534:THR:HG22	1:A:537:ALA:N	1.99	0.73
1:B:572:THR:HB	5:B:1789:HOH:O	1.87	0.73
1:A:478:MET:CE	1:A:793:LEU:HD22	2.18	0.73
1:A:543:THR:HG23	5:A:1707:HOH:O	1.90	0.71
1:B:534:THR:HG22	1:B:537:ALA:N	1.99	0.71
1:A:563:THR:HB	1:A:572:THR:HG22	1.73	0.70
1:B:563:THR:HB	1:B:572:THR:HG22	1.74	0.69
1:B:534:THR:HG23	1:B:649:GLU:OE1	1.94	0.68
1:B:339:LYS:HE3	5:B:1834:HOH:O	1.92	0.68
1:A:995:ILE:CG1	1:A:998:MET:CE	2.62	0.67
1:A:114:ASP:OD1	1:A:116:THR:HB	1.94	0.66
1:A:534:THR:HG23	1:A:649:GLU:OE1	1.95	0.65
1:B:543:THR:HG23	5:B:1641:HOH:O	1.97	0.64
1:A:478:MET:CE	3:A:1505:MVL:H6C2	2.26	0.64
1:B:534:THR:CG2	1:B:649:GLU:OE1	2.46	0.64
1:A:534:THR:CG2	1:A:649:GLU:OE1	2.47	0.63
1:A:236:LEU:HD12	1:A:236:LEU:O	2.00	0.61
1:A:417:SER:HB2	1:A:423:ARG:N	2.06	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:MET:CE	3:B:1505:MVL:H6C2	2.31	0.60
1:B:851:ASN:OD1	1:B:853:SER:HB2	2.01	0.59
1:A:851:ASN:OD1	1:A:853:SER:HB2	2.03	0.59
1:A:995:ILE:CG1	1:A:998:MET:HE3	2.26	0.59
1:A:98:SER:OG	1:A:126:ALA:HB1	2.03	0.58
1:B:1196:THR:OG1	1:B:1225:VAL:HG13	2.04	0.57
1:A:517:HIS:CD2	1:A:664:LYS:HB2	2.40	0.56
1:A:1333:MET:CE	5:A:1646:HOH:O	2.33	0.55
1:A:206:ASN:C	1:A:206:ASN:OD1	2.43	0.55
1:A:236:LEU:HD12	1:A:236:LEU:C	2.27	0.54
1:A:1009:TYR:CE2	1:A:1011:HIS:HB2	2.43	0.54
1:B:517:HIS:CD2	1:B:664:LYS:HB2	2.43	0.54
1:A:1198:SER:HB3	1:A:1223:SER:HB2	1.88	0.54
1:A:995:ILE:H	1:A:998:MET:HE1	1.69	0.53
1:B:248:LYS:HE3	1:B:457:ASN:O	2.09	0.53
1:A:995:ILE:N	1:A:998:MET:CE	2.55	0.52
1:A:1323:THR:O	1:A:1327:GLN:HG3	2.09	0.52
1:B:1198:SER:HB3	1:B:1223:SER:HB2	1.91	0.52
1:A:98:SER:HG	1:A:126:ALA:HB1	1.76	0.51
1:B:1009:TYR:CE2	1:B:1011:HIS:HB2	2.45	0.51
1:B:478:MET:CE	1:B:793:LEU:CD2	2.85	0.51
1:A:705:VAL:HG11	1:A:714:LYS:HD2	1.92	0.51
1:B:571:ILE:HD13	1:B:594:PHE:CE2	2.46	0.51
1:A:470:VAL:HG12	1:A:484:PHE:HB3	1.92	0.50
1:B:705:VAL:HG11	1:B:714:LYS:HD2	1.92	0.50
1:A:261:TYR:CE1	1:A:311:VAL:HG21	2.47	0.49
1:A:1255:VAL:HG22	1:A:1270:GLN:HG2	1.94	0.49
1:B:417:SER:HB2	1:B:423:ARG:H	1.78	0.49
1:B:470:VAL:HG12	1:B:484:PHE:HB3	1.94	0.48
1:A:291:SER:HB3	1:A:356:LYS:HG3	1.96	0.48
1:B:248:LYS:HE2	5:B:1639:HOH:O	2.12	0.48
1:A:534:THR:HG21	1:A:537:ALA:HB3	1.95	0.48
1:A:719:TYR:CZ	1:A:775:GLN:HG2	2.48	0.48
1:A:1345:PRO:O	1:A:1349:GLN:HG2	2.13	0.48
1:A:1225:VAL:HG22	1:A:1297:LYS:HG3	1.95	0.48
1:B:261:TYR:CE1	1:B:311:VAL:HG21	2.48	0.48
1:A:478:MET:CE	1:A:793:LEU:CD2	2.90	0.48
4:A:1506:B3P:O6	4:A:1506:B3P:C3	2.60	0.48
1:B:534:THR:HG21	1:B:537:ALA:HB3	1.93	0.48
1:A:803:PHE:HB2	1:A:819:PHE:CZ	2.48	0.48
1:A:1221:THR:N	1:A:1222:PRO:HD3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:747:TRP:HA	5:A:1674:HOH:O	2.14	0.47
1:B:311:VAL:HA	1:B:374:ALA:O	2.13	0.47
1:B:1345:PRO:O	1:B:1349:GLN:HG3	2.13	0.47
1:A:135:PRO:HA	1:A:196:TYR:O	2.14	0.47
1:B:1255:VAL:HG22	1:B:1270:GLN:HG2	1.96	0.47
1:B:478:MET:HE3	3:B:1505:MVL:C6	2.42	0.47
1:A:698:PRO:HG2	1:A:768:LEU:HD22	1.96	0.47
1:B:1014:GLN:HG3	1:B:1061:GLU:OE2	2.14	0.47
1:B:719:TYR:CZ	1:B:775:GLN:HG2	2.49	0.47
1:B:803:PHE:HB2	1:B:819:PHE:CZ	2.50	0.46
1:A:311:VAL:HA	1:A:374:ALA:O	2.15	0.46
1:B:48:SER:HB3	1:B:50:GLU:HG2	1.97	0.46
1:A:339:LYS:HE2	1:A:378:PRO:HG3	1.98	0.46
1:A:981:THR:O	1:A:1008:MET:HG2	2.15	0.46
1:B:588:LEU:HG	1:B:589:PHE:N	2.30	0.46
1:A:1360:HIS:HD2	1:A:1365:HIS:ND1	2.13	0.46
1:B:417:SER:CB	1:B:423:ARG:H	2.27	0.46
1:A:849:TYR:OH	1:A:924:GLY:HA2	2.17	0.45
1:B:858:LEU:HB3	1:B:941:ASP:HB3	1.99	0.45
1:A:957:ASP:OD1	1:A:1164:SER:HB3	2.17	0.45
1:A:146:ALA:HA	1:A:215:ALA:HB2	1.99	0.45
1:B:720:SER:OG	1:B:778:ASP:OD1	2.35	0.45
1:B:1066:TYR:C	1:B:1066:TYR:CD1	2.90	0.45
1:A:478:MET:HE3	1:A:793:LEU:CD2	2.47	0.44
4:B:1506:B3P:H112	4:B:1506:B3P:H21	1.60	0.44
1:A:58:TRP:CE2	1:A:276:LYS:HE3	2.53	0.44
1:A:720:SER:OG	1:A:778:ASP:OD1	2.35	0.44
1:B:437:ASN:CG	1:B:634:THR:HG21	2.36	0.44
1:B:1161:ILE:HD11	5:B:1838:HOH:O	2.17	0.44
1:B:56:LEU:HG	1:B:237:ILE:HG13	2.00	0.44
1:A:88:ILE:HD12	1:A:88:ILE:HA	1.62	0.44
1:B:466:GLN:O	1:B:467:ALA:HB2	2.19	0.43
1:B:957:ASP:OD1	1:B:1164:SER:HB3	2.17	0.43
1:A:543:THR:HG22	1:A:627:VAL:HB	2.00	0.43
1:A:1066:TYR:C	1:A:1066:TYR:CD1	2.92	0.43
1:B:396:LYS:HE3	1:B:396:LYS:HB2	1.82	0.43
1:A:858:LEU:HB3	1:A:941:ASP:HB3	2.00	0.43
1:B:79:VAL:HG23	1:B:79:VAL:O	2.18	0.43
1:B:1259:SER:HB2	1:B:1265:TRP:CE3	2.54	0.43
1:B:698:PRO:HG2	1:B:768:LEU:HD22	2.01	0.43
1:A:954:VAL:HG12	1:A:954:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1222:PRO:HD2	1:A:1300:ILE:HB	2.01	0.42
1:B:1214:GLN:HA	1:B:1312:ALA:HA	2.01	0.42
1:B:1222:PRO:HD2	1:B:1300:ILE:HB	2.01	0.42
1:A:582:SER:HA	1:A:787:SER:O	2.19	0.42
1:B:437:ASN:HD21	1:B:634:THR:CG2	2.32	0.42
1:B:849:TYR:OH	1:B:924:GLY:HA2	2.19	0.42
1:B:872:ALA:HB2	1:B:899:PHE:CB	2.49	0.42
1:B:1339:SER:O	1:B:1340:LYS:HB2	2.19	0.42
1:B:1373:LEU:O	1:B:1376:PHE:HB3	2.19	0.42
1:A:194:THR:HB	1:A:196:TYR:CE2	2.55	0.42
1:B:582:SER:HA	1:B:787:SER:O	2.20	0.42
1:A:1014:GLN:N	1:A:1015:PRO:CD	2.82	0.42
1:B:248:LYS:CE	5:B:1639:HOH:O	2.68	0.42
1:A:466:GLN:O	1:A:467:ALA:HB2	2.19	0.42
1:B:882:GLY:HA2	1:B:889:TYR:CE1	2.54	0.42
1:B:51:LYS:HD3	1:B:51:LYS:HA	1.81	0.41
1:A:1225:VAL:CG2	1:A:1297:LYS:HG3	2.51	0.41
1:B:954:VAL:HG12	1:B:954:VAL:O	2.21	0.41
1:A:754:TRP:N	1:A:755:PRO:HD2	2.35	0.41
1:A:1339:SER:O	1:A:1340:LYS:HB2	2.21	0.41
1:A:163:LEU:HD23	1:A:163:LEU:HA	1.87	0.41
1:B:769:ILE:HG12	1:B:803:PHE:CD1	2.56	0.41
1:B:975:LEU:O	1:B:978:PHE:HB3	2.21	0.41
1:B:1237:MET:HB2	1:B:1317:LEU:HB2	2.03	0.41
1:A:995:ILE:CG1	1:A:998:MET:HE2	2.20	0.41
1:A:1259:SER:HB2	1:A:1265:TRP:CE3	2.55	0.41
1:B:754:TRP:N	1:B:755:PRO:HD2	2.36	0.41
1:A:1214:GLN:HA	1:A:1312:ALA:HA	2.03	0.41
1:B:872:ALA:HB2	1:B:899:PHE:HB3	2.03	0.41
1:A:105:GLU:HA	1:A:118:LYS:O	2.21	0.40
1:A:75:ILE:CG2	1:A:76:ASP:N	2.84	0.40
1:A:588:LEU:HG	1:A:589:PHE:N	2.36	0.40
1:A:882:GLY:HA2	1:A:889:TYR:CE1	2.57	0.40
1:B:666:GLU:HG3	5:B:1733:HOH:O	2.22	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	1369/1411 (97%)	1312 (96%)	55 (4%)	2 (0%)	51	64
1	B	1220/1411 (86%)	1175 (96%)	44 (4%)	1 (0%)	51	64
All	All	2589/2822 (92%)	2487 (96%)	99 (4%)	3 (0%)	51	64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	743	ASN
1	B	743	ASN
1	A	794	MET

5.3.2 Protein sidechains (i)

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	1138/1178 (97%)	1096 (96%)	42 (4%)	34	48
1	B	1010/1178 (86%)	978 (97%)	32 (3%)	39	54
All	All	2148/2356 (91%)	2074 (97%)	74 (3%)	37	51

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ASP
1	A	88	ILE
1	A	116	THR

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Mol	Chain	Res	Type
1	A	119	TRP
1	A	128	ILE
1	A	134	GLU
1	A	164	ASP
1	A	190	LEU
1	A	194	THR
1	A	224	GLU
1	A	225	VAL
1	A	242	THR
1	A	329	VAL
1	A	379	LYS
1	A	417	SER
1	A	495	THR
1	A	534	THR
1	A	543	THR
1	A	548	THR
1	A	571	ILE
1	A	572	THR
1	A	588	LEU
1	A	598	VAL
1	A	601	SER
1	A	603	LYS
1	A	627	VAL
1	A	628	VAL
1	A	634	THR
1	A	692	TYR
1	A	705	VAL
1	A	720	SER
1	A	744	ASN
1	A	785	TRP
1	A	880	GLU
1	A	909	MET
1	A	953	HIS
1	A	1125	LYS
1	A	1139	ASN
1	A	1216	SER
1	A	1266	SER
1	A	1297	LYS
1	A	1308	VAL
1	B	41	SER
1	B	242	THR
1	B	329	VAL

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Mol	Chain	Res	Type
1	B	379	LYS
1	B	495	THR
1	B	534	THR
1	B	543	THR
1	B	548	THR
1	B	572	THR
1	B	578	LYS
1	B	588	LEU
1	B	598	VAL
1	B	601	SER
1	B	605	THR
1	B	622	LYS
1	B	627	VAL
1	B	628	VAL
1	B	634	THR
1	B	692	TYR
1	B	705	VAL
1	B	744	ASN
1	B	785	TRP
1	B	880	GLU
1	B	909	MET
1	B	953	HIS
1	B	1102	SER
1	B	1139	ASN
1	B	1216	SER
1	B	1225	VAL
1	B	1292	LYS
1	B	1331	GLU
1	B	1338	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1360	HIS
1	B	1351	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 9 are monoatomic - leaving 5 for Mogul analysis.

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	$\#\|Z\| > 2$
3	MVL	B	1505	2	13,15,15	0.94	1 (7%)	11,22,22	2.36	3 (27%)
4	B3P	B	1506	-	18,18,18	0.43	0	21,23,23	0.98	2 (9%)
3	MVL	A	1505	2	13,15,15	0.85	1 (7%)	11,22,22	2.41	4 (36%)
4	B3P	A	1506	-	18,18,18	0.47	0	21,23,23	0.92	1 (4%)
3	MVL	A	1508	-	13,15,15	0.43	0	11,22,22	1.47	2 (18%)

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
3	MVL	B	1505	2	-	0/2/22/22	0/1/2/2
4	B3P	B	1506	-	-	18/28/28/28	-
3	MVL	A	1505	2	-	1/2/22/22	0/1/2/2
4	B3P	A	1506	-	-	17/28/28/28	-
3	MVL	A	1508	-	-	2/2/22/22	0/1/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1505	MVL	C1-C2	-2.79	1.47	1.51
3	A	1505	MVL	C1-C2	-2.03	1.48	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1505	MVL	C4-C3-C2	5.28	118.26	110.24
3	A	1505	MVL	C4-C3-C2	4.79	117.51	110.24
3	A	1505	MVL	C6-C5-C4	-4.25	104.78	112.45
3	B	1505	MVL	C8-N10-C1	-3.96	105.30	109.05
3	A	1505	MVL	C8-N10-C1	-3.78	105.48	109.05
3	A	1508	MVL	C8-N10-C1	-3.48	105.76	109.05
3	B	1505	MVL	C6-C5-C4	-2.80	107.39	112.45
3	A	1508	MVL	C6-C5-C4	-2.73	107.52	112.45
4	B	1506	B3P	O5-C6-C4	2.26	116.22	111.63
4	B	1506	B3P	O4-C5-C4	2.25	116.20	111.63
3	A	1505	MVL	C3-C4-C5	2.19	115.07	111.37
4	A	1506	B3P	O4-C5-C4	2.09	115.86	111.63

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1506	B3P	N1-C4-C6-O5
4	A	1506	B3P	C5-C4-C6-O5
4	A	1506	B3P	C7-C4-C6-O5
4	A	1506	B3P	N1-C4-C7-O6
4	A	1506	B3P	C5-C4-C7-O6
4	A	1506	B3P	C6-C4-C7-O6
4	A	1506	B3P	C9-C8-N2-C2
4	A	1506	B3P	C10-C8-N2-C2
4	A	1506	B3P	C11-C8-N2-C2
4	A	1506	B3P	O2-C10-C8-N2
4	A	1506	B3P	O2-C10-C8-C9
4	A	1506	B3P	O2-C10-C8-C11
4	B	1506	B3P	C5-C4-N1-C3
4	B	1506	B3P	C6-C4-N1-C3
4	B	1506	B3P	C7-C4-N1-C3
4	B	1506	B3P	N1-C4-C5-O4
4	B	1506	B3P	C6-C4-C5-O4
4	B	1506	B3P	C7-C4-C5-O4
4	B	1506	B3P	N1-C4-C6-O5

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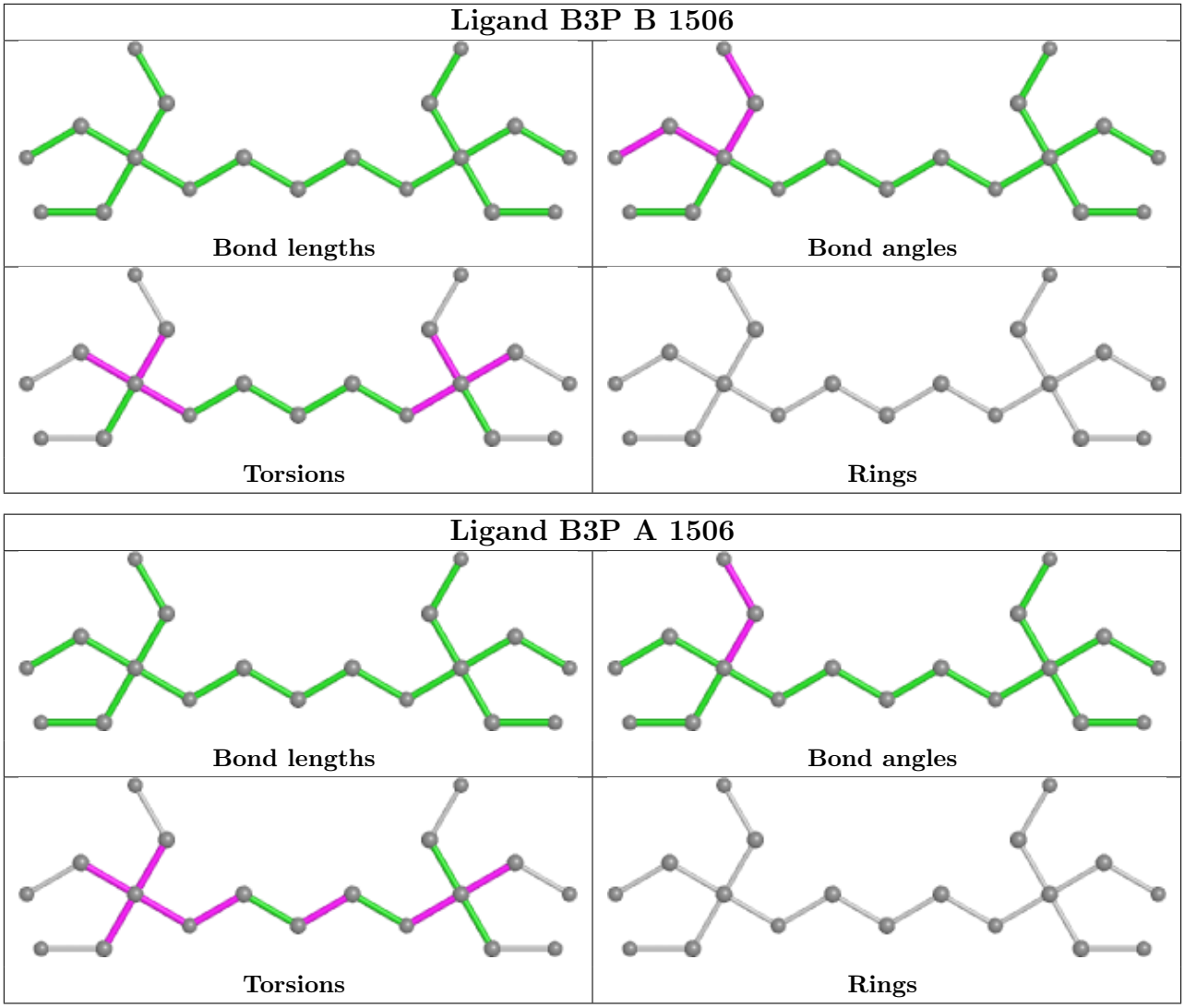
Mol	Chain	Res	Type	Atoms
4	B	1506	B3P	C5-C4-C6-O5
4	B	1506	B3P	C7-C4-C6-O5
4	B	1506	B3P	C10-C8-N2-C2
4	B	1506	B3P	C11-C8-N2-C2
4	B	1506	B3P	O2-C10-C8-N2
4	B	1506	B3P	O2-C10-C8-C9
4	B	1506	B3P	O2-C10-C8-C11
4	B	1506	B3P	O3-C11-C8-N2
4	B	1506	B3P	O3-C11-C8-C9
4	B	1506	B3P	O3-C11-C8-C10
4	A	1506	B3P	C6-C4-C5-O4
4	A	1506	B3P	C1-C3-N1-C4
4	A	1506	B3P	C7-C4-N1-C3
3	A	1508	MVL	C4-C5-C6-O6
3	A	1508	MVL	N10-C5-C6-O6
4	B	1506	B3P	C9-C8-N2-C2
4	A	1506	B3P	N1-C4-C5-O4
4	A	1506	B3P	C3-C1-C2-N2
3	A	1505	MVL	N10-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1505	MVL	3	0
4	B	1506	B3P	1	0
3	A	1505	MVL	2	0
4	A	1506	B3P	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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, 95^{th} 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	1371/1411 (97%)	-0.37	4 (0%)	94	96	16, 28, 50, 80	0
1	B	1224/1411 (86%)	-0.17	14 (1%)	80	85	16, 32, 65, 112	0
All	All	2595/2822 (91%)	-0.27	18 (0%)	87	91	16, 30, 58, 112	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	227	ALA	5.5
1	A	566	ALA	3.2
1	B	652	LEU	3.2
1	A	567	LYS	3.1
1	B	1372	HIS	2.9
1	B	653	ASN	2.7
1	A	492	THR	2.6
1	B	1385	LEU	2.5
1	B	228	PRO	2.5
1	B	1307	GLU	2.5
1	A	227	ALA	2.4
1	B	1302	GLU	2.3
1	B	1267	VAL	2.3
1	B	1216	SER	2.2
1	B	79	VAL	2.2
1	B	1197	VAL	2.2
1	B	1248	ASN	2.1
1	B	1218	LYS	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 (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

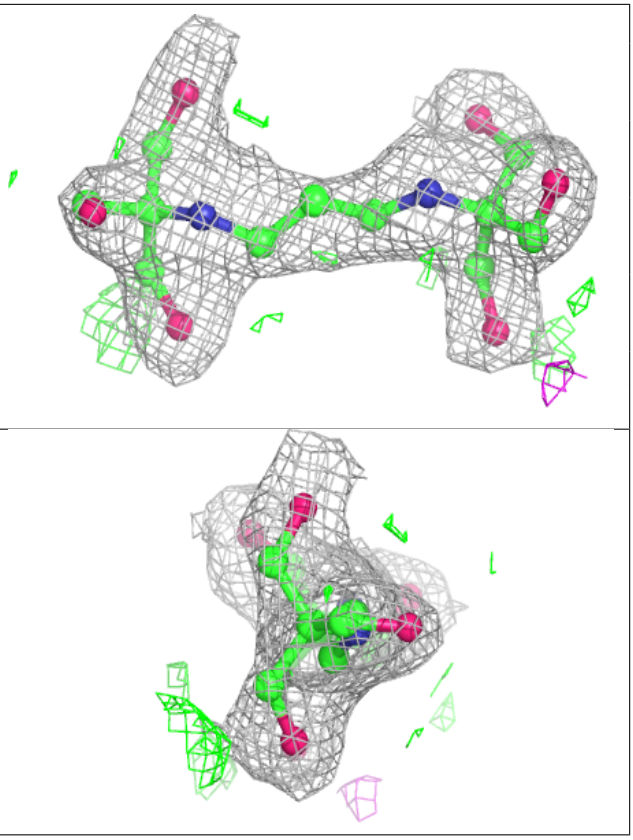
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	B3P	A	1506	19/19	0.89	0.15	37,50,60,61	0
4	B3P	B	1506	19/19	0.89	0.15	36,49,77,78	0
2	CA	B	1503	1/1	0.94	0.06	54,54,54,54	0
2	CA	A	1503	1/1	0.95	0.04	39,39,39,39	0
3	MVL	A	1508	14/14	0.96	0.12	28,38,42,46	0
2	CA	A	1504	1/1	0.96	0.11	21,21,21,21	0
3	MVL	A	1505	14/14	0.96	0.18	25,26,28,30	0
3	MVL	B	1505	14/14	0.98	0.14	20,22,26,27	0
2	CA	B	1502	1/1	0.98	0.06	24,24,24,24	0
2	CA	B	1504	1/1	0.98	0.06	36,36,36,36	0
2	CA	A	1507	1/1	0.99	0.05	25,25,25,25	0
2	CA	A	1501	1/1	0.99	0.11	25,25,25,25	0
2	CA	A	1502	1/1	0.99	0.08	29,29,29,29	0
2	CA	B	1501	1/1	1.00	0.09	22,22,22,22	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

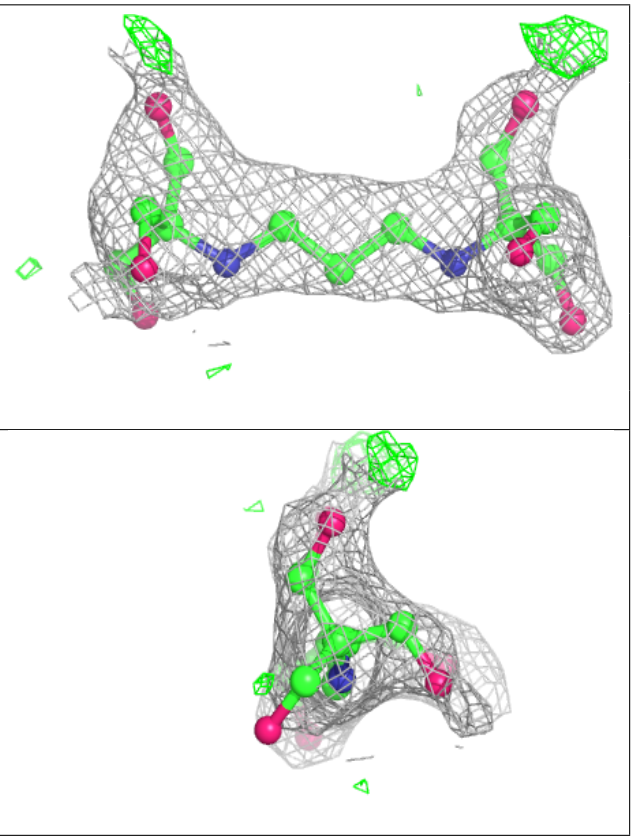
Electron density around B3P A 1506:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around B3P B 1506:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.