



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:19 PM UTC

PDB ID : 7NSN / pdb_00007nsn
Title : Multi-domain GH92 alpha-1,2-mannosidase from *Neobacillus novalis*: mannoimidazole complex
Authors : Kolaczowski, 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

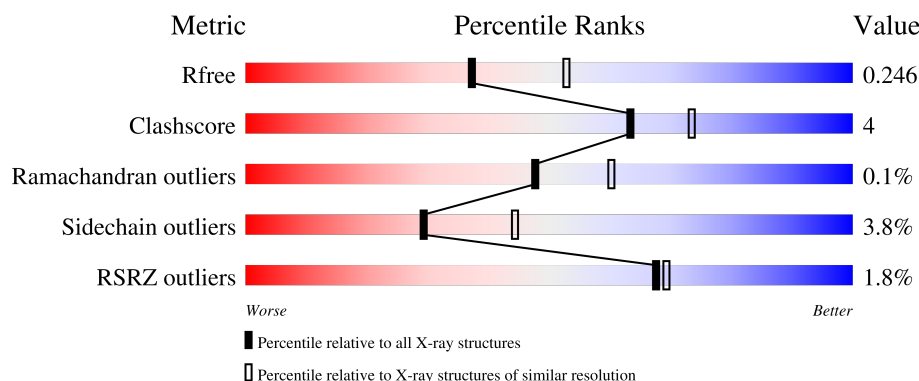
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.29 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 $\leq 5\%$. 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	1411	86% 10% ...
1	B	1411	3% 77% 9% 13%

2 Entry composition [i](#)

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.

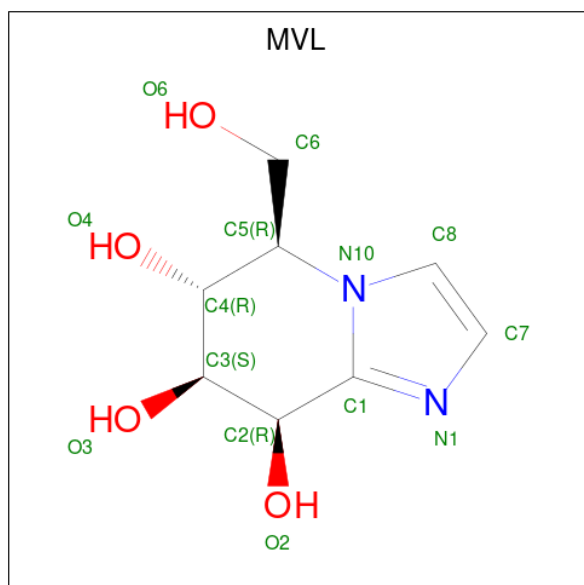
- Molecule 1 is a protein called GH92 alpha-1,2-mannosidase.

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 (CCD ID: CA) (formula: Ca).

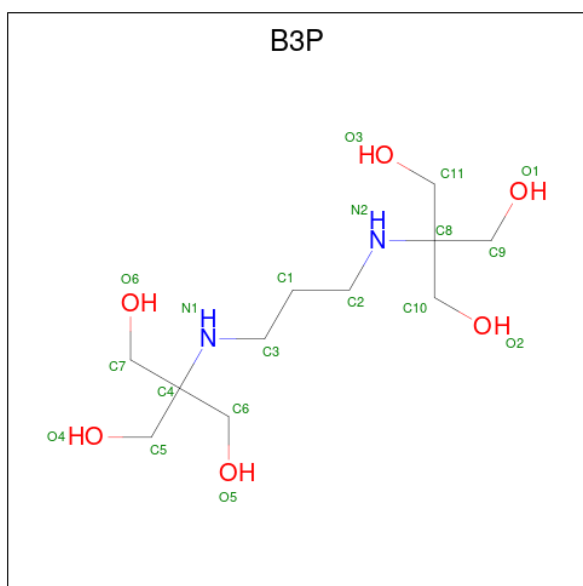
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total	Ca	0	0
			5	5		
2	B	4	Total	Ca	0	0
			4	4		

- Molecule 3 is (5R,6R,7S,8R)-5-(HYDROXYMETHYL)-5,6,7,8-TETRAHYDROIMIDAZO[1,2-A]PYRIDINE-6,7,8-TRIOL (CCD ID: MVL) (formula: C₈H₁₂N₂O₄).



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)-PROPYLAMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: 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

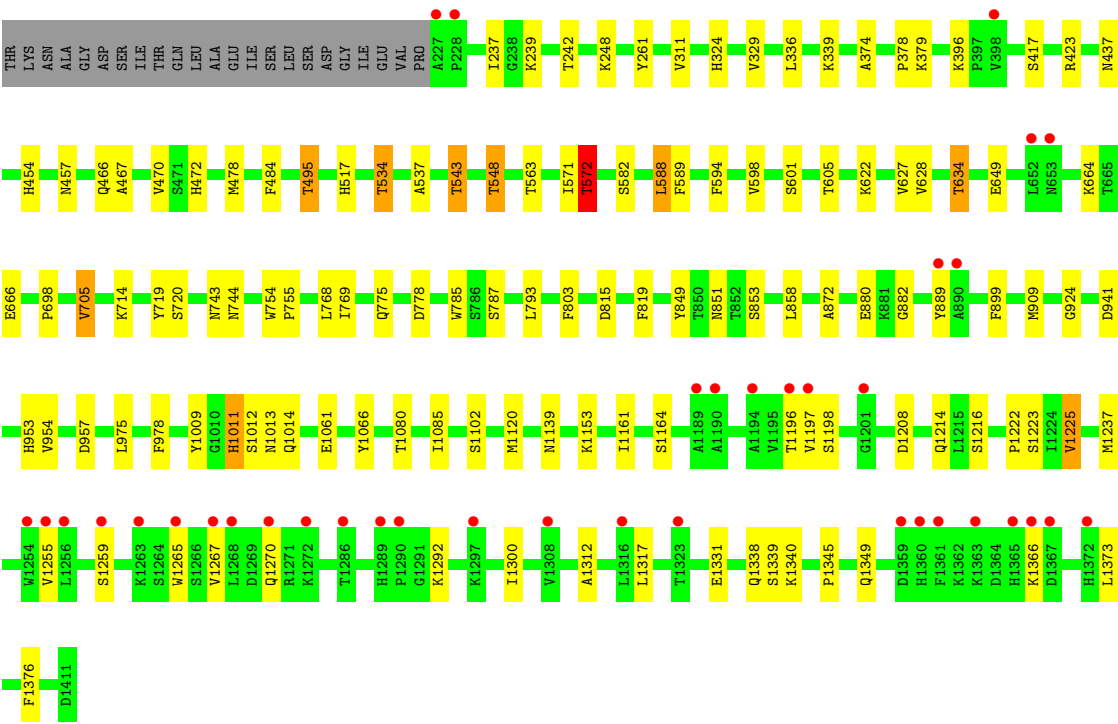
- Molecule 5 is water.

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

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.

- Chain A: 
- | Position | Residue | Conservation |
|----------|---------|--------------|
| 1 | Q924 | High |
| 2 | W1265 | High |
| 3 | D941 | High |
| 4 | Q1270 | High |
| 5 | H953 | High |
| 6 | K1297 | High |
| 7 | Y954 | High |
| 8 | D957 | High |
| 9 | T1300 | High |
| 10 | V1308 | High |
| 11 | A1312 | High |
| 12 | D1321 | High |
| 13 | V1322 | High |
| 14 | T1323 | High |
| 15 | Q1327 | High |
| 16 | M1333 | High |
| 17 | Q1338 | High |
| 18 | S1339 | High |
| 19 | K1340 | High |
| 20 | P1345 | High |
| 21 | Q1349 | High |
| 22 | H1360 | High |
| 23 | H1365 | High |
| 24 | D1375 | High |
| 25 | D1411 | High |
| 26 | L852 | High |
| 27 | M853 | High |
| 28 | K664 | High |
| 29 | D682 | High |
| 30 | P698 | High |
| 31 | V705 | High |
| 32 | K714 | High |
| 33 | P718 | High |
| 34 | Y719 | High |
| 35 | S720 | High |
| 36 | M1008 | High |
| 37 | Y1009 | High |
| 38 | G1010 | High |
| 39 | H1011 | High |
| 40 | S1012 | High |
| 41 | N1013 | High |
| 42 | Q1014 | High |
| 43 | P1015 | High |
| 44 | Y1066 | High |
| 45 | T1080 | High |
| 46 | I1085 | High |
| 47 | M1120 | High |
| 48 | K1121 | High |
| 49 | K1125 | High |
| 50 | H1139 | High |
| 51 | E1146 | High |
| 52 | S1164 | High |
| 53 | D1185 | High |
| 54 | S1198 | High |
| 55 | D1208 | High |
| 56 | Q1214 | High |
| 57 | L1215 | High |
| 58 | S1216 | High |
| 59 | T1221 | High |
| 60 | P1222 | High |
| 61 | S1223 | High |
| 62 | I1224 | High |
| 63 | V1225 | High |
| 64 | V1255 | High |
| 65 | S1269 | High |
| 66 | R385 | High |
| 67 | S417 | High |
| 68 | R423 | High |
| 69 | N437 | High |
| 70 | H454 | High |
| 71 | Q466 | High |
| 72 | A467 | High |
| 73 | V470 | High |
| 74 | M478 | High |
| 75 | F484 | High |
| 76 | T495 | High |
| 77 | H517 | High |
| 78 | T534 | High |
| 79 | D535 | High |
| 80 | H536 | High |
| 81 | A537 | High |
| 82 | T543 | High |
| 83 | T548 | High |
| 84 | T563 | High |
| 85 | W785 | High |
| 86 | S786 | High |
| 87 | S787 | High |
| 88 | L571 | High |
| 89 | M794 | High |
| 90 | F803 | High |
| 91 | F819 | High |
| 92 | Y849 | High |
| 93 | N851 | High |
| 94 | T850 | High |
| 95 | S852 | High |
| 96 | G802 | High |
| 97 | K603 | High |
| 98 | L858 | High |
| 99 | V627 | High |
| 100 | V628 | High |
| 101 | K881 | High |
| 102 | G882 | High |
| 103 | Y889 | High |
| 104 | M909 | High |
| 105 | E640 | High |
| 106 | E649 | High |
| 107 | T117 | High |
| 108 | K118 | High |
| 109 | A126 | High |
| 110 | N127 | High |
| 111 | I128 | High |
| 112 | E134 | High |
| 113 | P136 | High |
| 114 | A146 | High |
| 115 | P154 | High |
| 116 | Y160 | High |
| 117 | L163 | High |
| 118 | D164 | High |
| 119 | T194 | High |
| 120 | K195 | High |
| 121 | Y196 | High |
| 122 | K200 | High |
| 123 | N206 | High |
| 124 | A215 | High |
| 125 | E224 | High |
| 126 | V225 | High |
| 127 | P226 | High |
| 128 | A227 | High |
| 129 | L236 | High |
| 130 | T242 | High |
| 131 | Y261 | High |
| 132 | K276 | High |
| 133 | S291 | High |
| 134 | V311 | High |
| 135 | V329 | High |
| 136 | L336 | High |
| 137 | K339 | High |
| 138 | K356 | High |
| 139 | A374 | High |
| 140 | P378 | High |
| 141 | K379 | High |
| 142 | S41 | High |
| 143 | W58 | High |
| 144 | T61 | High |
| 145 | I75 | High |
| 146 | D76 | High |
| 147 | V79 | High |
| 148 | I88 | High |
| 149 | S98 | High |
| 150 | E106 | High |
| 151 | D114 | High |
| 152 | P115 | High |
| 153 | F116 | High |

- [illegible]



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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)	0.33 , 27.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.63	2/10900 (0.0%)	1.12	17/14803 (0.1%)
1	B	0.63	3/9721 (0.0%)	1.11	14/13195 (0.1%)
All	All	0.63	5/20621 (0.0%)	1.12	31/27998 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1011	HIS	CE1-NE2	5.85	1.38	1.32
1	A	1011	HIS	CE1-NE2	5.66	1.38	1.32
1	A	536	HIS	CE1-NE2	5.42	1.38	1.32
1	B	324	HIS	CE1-NE2	5.29	1.37	1.32
1	B	472	HIS	CE1-NE2	5.17	1.37	1.32

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	THR	CA-CB-OG1	-7.01	99.08	109.60
1	B	64	THR	CA-CB-OG1	-6.90	99.26	109.60
1	A	1365	HIS	CA-CB-CG	6.25	120.05	113.80
1	B	495	THR	CA-CB-OG1	-5.98	100.63	109.60
1	B	44	ASP	CA-CB-CG	5.84	118.44	112.60
1	A	160	TYR	CA-C-N	5.84	126.21	122.18
1	A	160	TYR	C-N-CA	5.84	126.21	122.18
1	B	548	THR	CA-CB-OG1	-5.81	100.89	109.60
1	A	1146	GLU	CB-CG-CD	5.61	122.13	112.60
1	B	65	ASP	CA-CB-CG	5.59	118.19	112.60
1	A	1185	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	572	THR	CA-CB-OG1	-5.56	101.27	109.60
1	A	718	PRO	CB-CA-C	5.51	116.17	110.00
1	B	815	ASP	CA-CB-CG	5.50	118.10	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1080	THR	CB-CA-C	5.49	117.43	109.20
1	A	154	PRO	CB-CA-C	-5.48	104.22	111.23
1	B	572	THR	CA-CB-OG1	-5.39	101.52	109.60
1	A	116	THR	CA-CB-OG1	-5.24	101.74	109.60
1	B	1208	ASP	CA-CB-CG	5.21	117.81	112.60
1	A	1321	ASP	CA-CB-CG	5.21	117.81	112.60
1	B	378	PRO	N-CA-C	5.18	120.58	113.84
1	B	1013	ASN	CA-C-N	5.17	126.55	120.09
1	B	1013	ASN	C-N-CA	5.17	126.55	120.09
1	B	454	HIS	CA-C-N	5.16	127.45	120.38
1	B	454	HIS	C-N-CA	5.16	127.45	120.38
1	A	737	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	454	HIS	CA-C-N	5.08	127.34	120.38
1	A	454	HIS	C-N-CA	5.08	127.34	120.38
1	B	1080	THR	CB-CA-C	5.08	116.81	109.45
1	A	1375	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	1208	ASP	CA-CB-CG	5.01	117.61	112.60

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	87	0
1	B	9492	0	9068	69	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	2	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	158	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 (158) 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:H	1:A:998:MET:HE3	1.08	1.17
1:A:995:ILE:HG12	1:A:998:MET:HE2	1.26	1.14
1:B:478:MET:HE1	1:B:793:LEU:HD22	1.31	1.12
1:A:478:MET:HE3	3:A:1505:MVL:H6C2	1.32	1.11
1:A:478:MET:HE1	1:A:793:LEU:HD22	1.34	1.06
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	1.58	1.02
1:B:478:MET:HE3	3:B:1505:MVL:H6C2	1.41	1.01
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	1.89	0.86
1:B:478:MET:HE1	1:B:793:LEU:CD2	2.09	0.81
1:A:682:ASP:HB3	5:A:1913:HOH:O	1.81	0.80
1:A:478:MET:HE1	1:A:793:LEU:CD2	2.14	0.78
1:A:995:ILE:HG12	1:A:998:MET:HE3	1.63	0.75
1:B:478:MET:CE	1:B:793:LEU:HD22	2.14	0.74
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:478:MET:HE3	3:B:1505:MVL:C6	2.21	0.69
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:98:SER:OG	1:A:126:ALA:HB1	2.03	0.58
1:A:236:LEU:HD12	1:A:236:LEU:C	2.27	0.58
1:B:1196:THR:OG1	1:B:1225:VAL:HG13	2.04	0.57
1:A:995:ILE:CG1	1:A:998:MET:HE3	2.28	0.57
1:A:206:ASN:C	1:A:206:ASN:OD1	2.43	0.57
1:A:517:HIS:CD2	1:A:664:LYS:HB2	2.40	0.56
1:B:1085:ILE:HD13	1:B:1120:MET:HE1	1.88	0.55
1:A:1333:MET:CE	5:A:1646:HOH:O	2.33	0.55
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: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: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:995:ILE:H	1:A:998:MET:HE1	1.72	0.50
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:1066:TYR:C	1:B:1066:TYR:CD1	2.90	0.49
1:B:478:MET:CE	1:B:793:LEU:CD2	2.85	0.49
1:B:417:SER:HB2	1:B:423:ARG:H	1.78	0.49
1:B:437:ASN:CG	1:B:634:THR:HG21	2.36	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:A:1085:ILE:HD13	1:A:1120:MET:HE1	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1066:TYR:C	1:A:1066:TYR:CD1	2.92	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
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: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
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: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:A:478:MET:HE3	3:A:1505:MVL:C6	2.23	0.43
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:995:ILE:CG1	1:A:998:MET:HE2	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:437:ASN:CG	1:A:634:THR:HG21	2.40	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: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:B:1339:SER:O	1:B:1340:LYS:HB2	2.19	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: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:478:MET:CE	1:A:793:LEU:CD2	2.90	0.40
1:A:747:TRP:CZ3	1:A:794:MET:HE2	2.56	0.40
1:B:1014:GLN:HG3	1:B:1061:GLU:CD	2.45	0.40
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

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	1369/1411 (97%)	1312 (96%)	55 (4%)	2 (0%)	48	60
1	B	1220/1411 (86%)	1175 (96%)	44 (4%)	1 (0%)	48	60
All	All	2589/2822 (92%)	2487 (96%)	99 (4%)	3 (0%)	48	60

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

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%)	1093 (96%)	45 (4%)	28	42
1	B	1010/1178 (86%)	973 (96%)	37 (4%)	30	45
All	All	2148/2356 (91%)	2066 (96%)	82 (4%)	29	44

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	VAL
1	A	88	ILE
1	A	116	THR

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Mol	Chain	Res	Type
1	A	128	ILE
1	A	134	GLU
1	A	136	VAL
1	A	164	ASP
1	A	194	THR
1	A	200	LYS
1	A	224	GLU
1	A	225	VAL
1	A	242	THR
1	A	329	VAL
1	A	336	LEU
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	640	GLU
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	1012	SER
1	A	1121	LYS
1	A	1125	LYS
1	A	1139	ASN
1	A	1216	SER
1	A	1297	LYS
1	A	1308	VAL
1	A	1338	GLN

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Mol	Chain	Res	Type
1	B	41	SER
1	B	239	LYS
1	B	242	THR
1	B	329	VAL
1	B	336	LEU
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	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	705	VAL
1	B	744	ASN
1	B	785	TRP
1	B	880	GLU
1	B	909	MET
1	B	953	HIS
1	B	1012	SER
1	B	1102	SER
1	B	1139	ASN
1	B	1153	LYS
1	B	1197	VAL
1	B	1216	SER
1	B	1225	VAL
1	B	1267	VAL
1	B	1292	LYS
1	B	1331	GLU
1	B	1338	GLN
1	B	1366	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN

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Mol	Chain	Res	Type
1	A	104	ASN
1	A	127	ASN
1	A	304	ASN
1	A	341	GLN
1	A	464	GLN
1	A	833	ASN
1	A	1106	ASN
1	A	1163	GLN
1	A	1273	ASN
1	A	1280	GLN
1	A	1349	GLN
1	A	1360	HIS
1	B	250	ASN
1	B	304	ASN
1	B	341	GLN
1	B	416	GLN
1	B	1163	GLN
1	B	1351	ASN
1	B	1402	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	A	1508	-	14,15,15	1.09	2 (14%)	14,22,22	1.26	1 (7%)
4	B3P	A	1506	-	18,18,18	0.48	0	23,23,23	0.87	1 (4%)
3	MVL	B	1505	2	14,15,15	0.86	1 (7%)	14,22,22	2.00	3 (21%)
3	MVL	A	1505	2	14,15,15	1.00	1 (7%)	14,22,22	2.19	4 (28%)
4	B3P	B	1506	-	18,18,18	0.44	0	23,23,23	0.98	2 (8%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1505	MVL	C1-N1	3.24	1.36	1.32
3	A	1508	MVL	C1-N1	3.01	1.36	1.32
3	A	1508	MVL	C1-N10	2.52	1.40	1.36
3	B	1505	MVL	C1-N1	2.50	1.35	1.32

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1505	MVL	C6-C5-C4	-5.41	104.78	112.93
3	B	1505	MVL	C4-C3-C2	5.09	118.26	110.22
3	A	1505	MVL	C4-C3-C2	4.61	117.51	110.22
3	B	1505	MVL	C6-C5-C4	-3.68	107.39	112.93
3	A	1508	MVL	C6-C5-C4	-3.59	107.52	112.93
3	B	1505	MVL	O3-C3-C2	-2.26	105.16	109.64
4	B	1506	B3P	O5-C6-C4	2.23	116.22	111.68
4	B	1506	B3P	O4-C5-C4	2.22	116.20	111.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1505	MVL	C3-C4-C5	2.19	115.07	111.37
4	A	1506	B3P	O4-C5-C4	2.06	115.86	111.68
3	A	1505	MVL	O3-C3-C2	-2.06	105.57	109.64

There are no chirality outliers.

All (37) 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
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	N10-C5-C6-O6
3	A	1508	MVL	C4-C5-C6-O6

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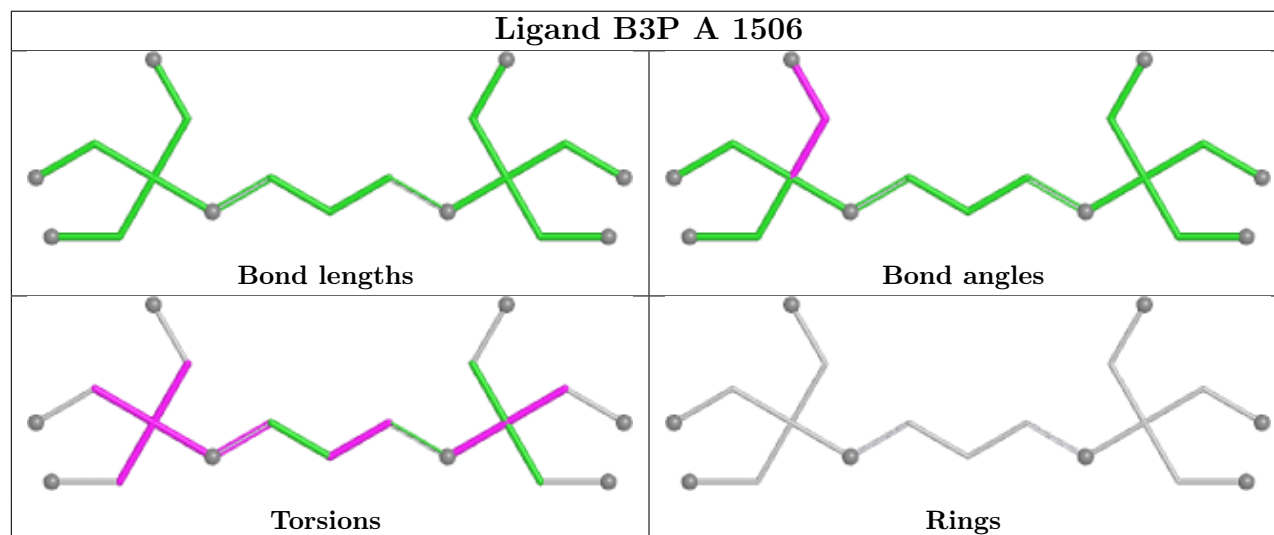
Mol	Chain	Res	Type	Atoms
4	B	1506	B3P	C9-C8-N2-C2
4	A	1506	B3P	N1-C4-C5-O4
4	A	1506	B3P	C3-C1-C2-N2

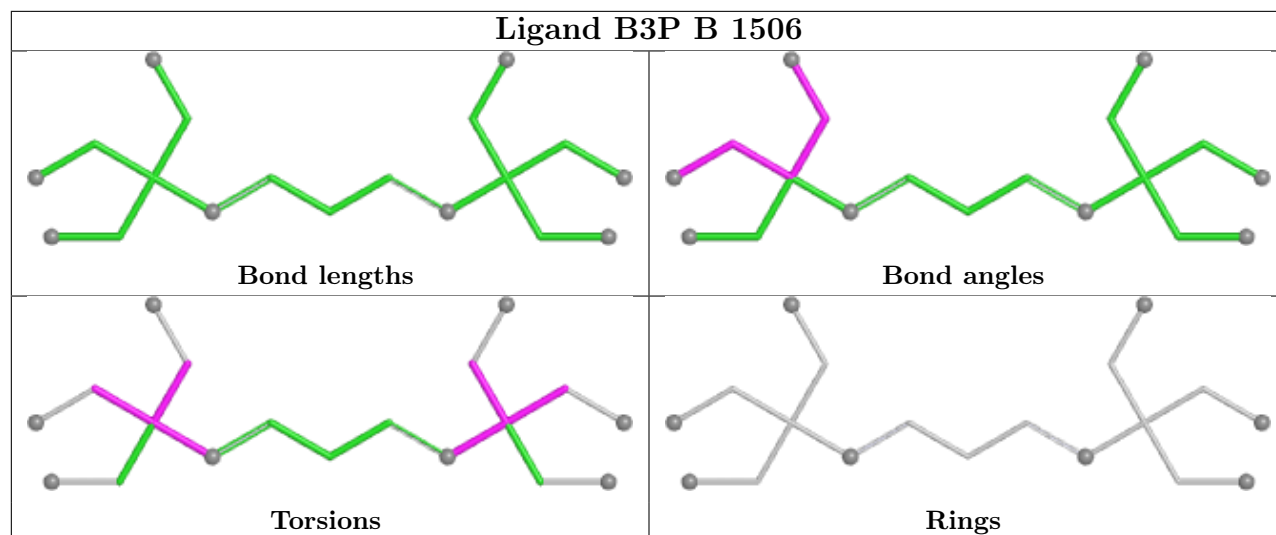
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1506	B3P	1	0
3	B	1505	MVL	2	0
3	A	1505	MVL	2	0
4	B	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 than 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1371/1411 (97%)	-0.42	8 (0%) 85 86	16, 28, 50, 80	0
1	B	1224/1411 (86%)	-0.06	40 (3%) 49 51	16, 32, 65, 112	0
All	All	2595/2822 (91%)	-0.25	48 (1%) 67 69	16, 30, 58, 112	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	652	LEU	4.2
1	A	225	VAL	4.2
1	B	79	VAL	3.8
1	B	1365	HIS	3.7
1	B	1267	VAL	3.6
1	B	1289	HIS	3.5
1	B	227	ALA	3.3
1	B	652	LEU	3.3
1	A	566	ALA	3.3
1	B	1372	HIS	3.2
1	B	1259	SER	3.1
1	B	398	VAL	3.1
1	B	1196	THR	3.0
1	B	1366	LYS	2.8
1	B	1255	VAL	2.8
1	B	1190	ALA	2.6
1	B	653	ASN	2.6
1	A	226	PRO	2.6
1	B	1360	HIS	2.6
1	B	1363	LYS	2.6
1	A	567	LYS	2.6
1	B	1286	THR	2.6
1	B	66	ALA	2.5
1	B	1361	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1367	ASP	2.5
1	B	1201	GLY	2.5
1	B	1265	TRP	2.5
1	B	1268	LEU	2.5
1	B	1323	THR	2.4
1	B	1194	ALA	2.4
1	B	1270	GLN	2.4
1	B	1263	LYS	2.3
1	B	1272	LYS	2.3
1	B	1308	VAL	2.2
1	A	227	ALA	2.2
1	B	1189	ALA	2.1
1	B	1316	LEU	2.1
1	A	653	ASN	2.1
1	B	1290	PRO	2.1
1	B	889	TYR	2.1
1	B	1197	VAL	2.1
1	B	1359	ASP	2.1
1	B	228	PRO	2.1
1	B	1254	TRP	2.1
1	A	224	GLU	2.0
1	B	1297	LYS	2.0
1	B	890	ALA	2.0
1	B	1256	LEU	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](#)

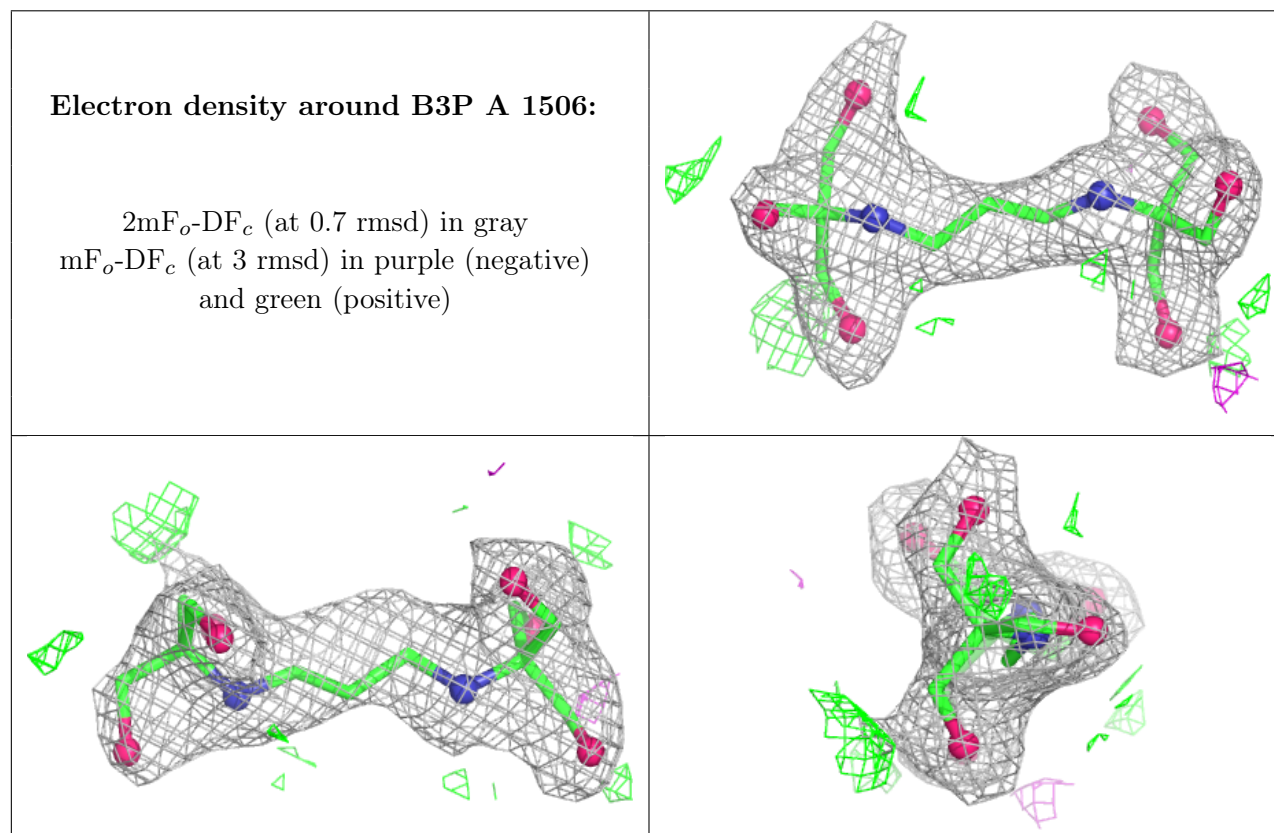
There are no oligosaccharides in this entry.

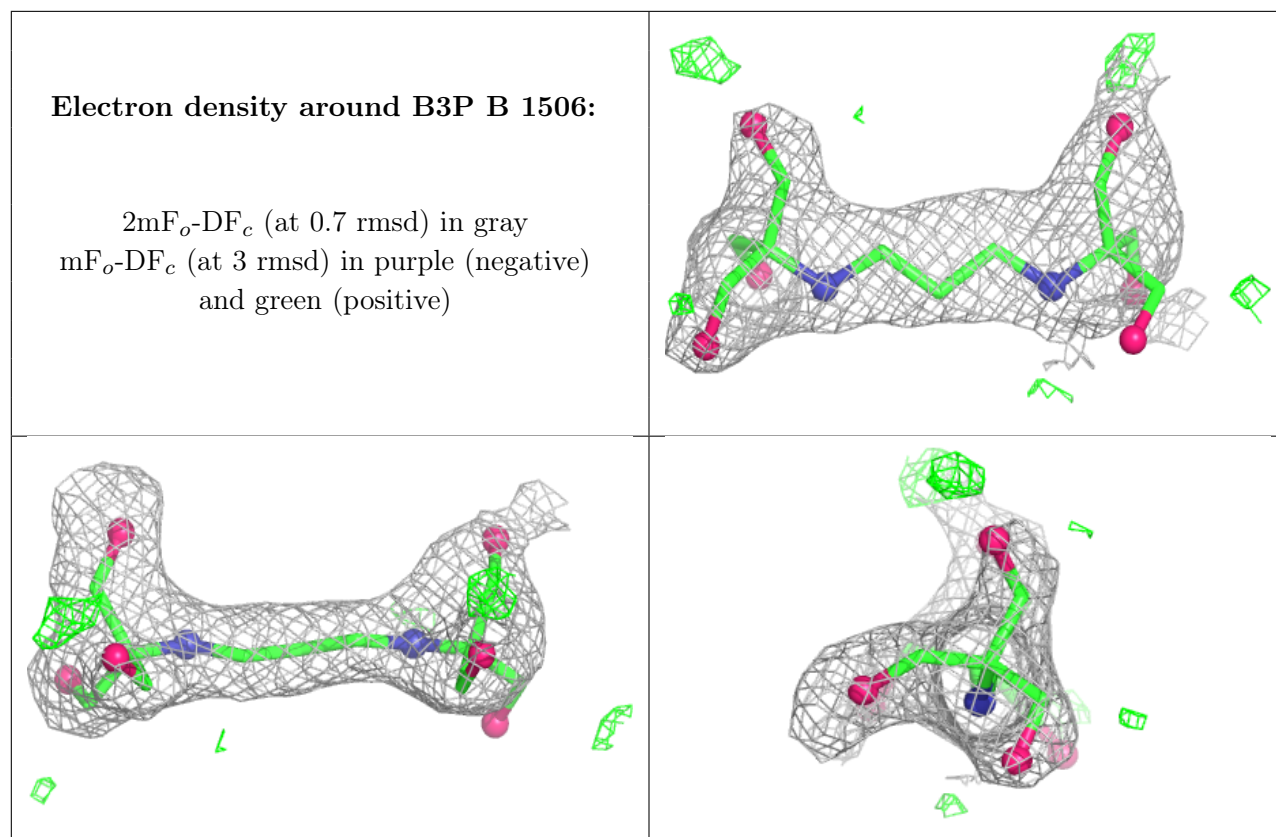
6.4 Ligands [i](#)

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, 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($\text{\AA}^2$)	Q<0.9
4	B3P	A	1506	19/19	0.87	0.13	37,50,60,61	0
4	B3P	B	1506	19/19	0.87	0.14	36,49,77,78	0
2	CA	B	1503	1/1	0.93	0.07	54,54,54,54	0
3	MVL	A	1508	14/14	0.95	0.07	28,38,42,46	0
3	MVL	A	1505	14/14	0.97	0.06	25,26,28,30	0
2	CA	A	1503	1/1	0.97	0.05	39,39,39,39	0
2	CA	A	1502	1/1	0.98	0.03	29,29,29,29	0
3	MVL	B	1505	14/14	0.98	0.05	20,22,26,27	0
2	CA	B	1504	1/1	0.98	0.04	36,36,36,36	0
2	CA	B	1502	1/1	0.98	0.03	24,24,24,24	0
2	CA	A	1504	1/1	0.99	0.04	21,21,21,21	0
2	CA	A	1507	1/1	0.99	0.02	25,25,25,25	0
2	CA	A	1501	1/1	1.00	0.04	25,25,25,25	0
2	CA	B	1501	1/1	1.00	0.02	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.