Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 04:24 am BST

PDB ID	:	4FS9
Title	:	Complex structure of a broad specificity amino acid racemase (Bar) within the reactive intermediate
Authors	:	Wang, W.C.; Wu, H.M.
Deposited on	:	2012-06-27
Resolution	:	3.10 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:

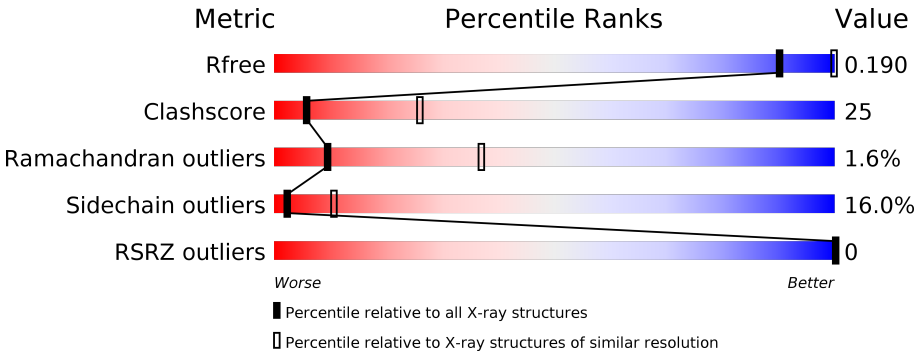
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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% 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	409	53% 33% 8% 6%
1	B	409	48% 41% 5% 6%

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	PE1	A	501	-	-	X	-
2	PE1	B	501	-	-	X	-

2 Entry composition

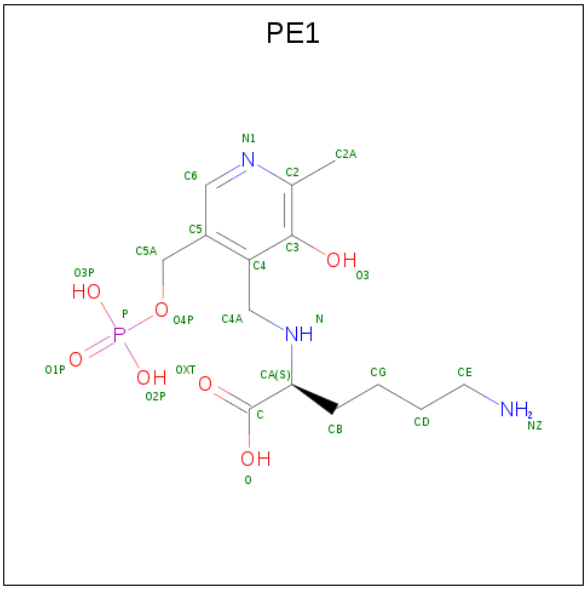
There are 3 unique types of molecules in this entry. The entry contains 5985 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Broad specificity amino acid racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			2920	1822	529	555	14			
1	B	384	Total	C	N	O	S	0	0	0
			2920	1822	529	555	14			

- Molecule 2 is N 2 -({3-HYDROXY-2-METHYL-5-[(PHOSPHONOOXY)METHYL]PYRIDIN-4-YL}METHYL)-L-LYSINE (three-letter code: PE1) (formula: $C_{14}H_{24}N_3O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	14	3	7	1		
2	B	1	Total	C	N	O	P	0	0
			25	14	3	7	1		

- Molecule 3 is water.

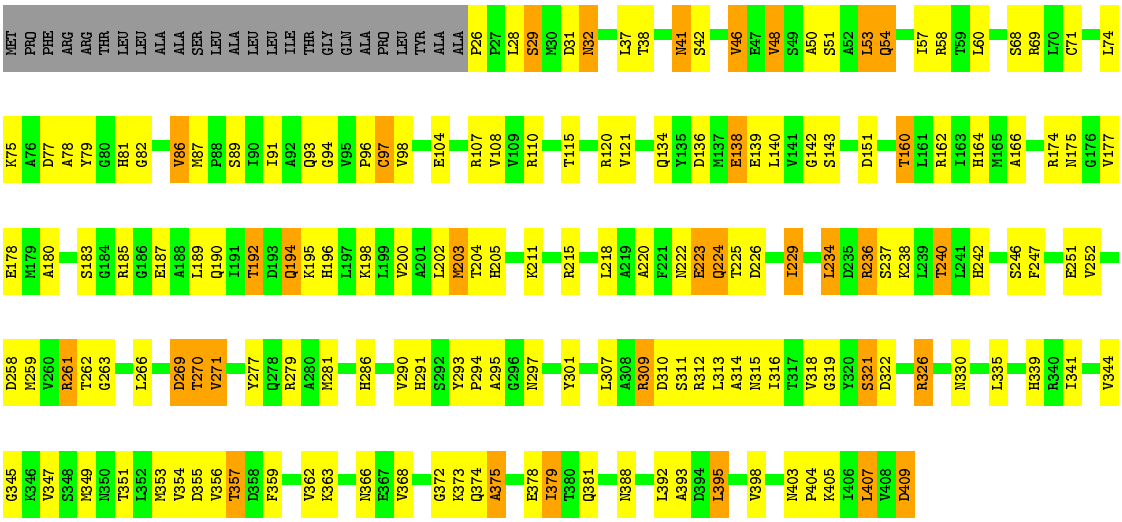
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	48	Total O 48 48	0	0
3	B	47	Total O 47 47	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

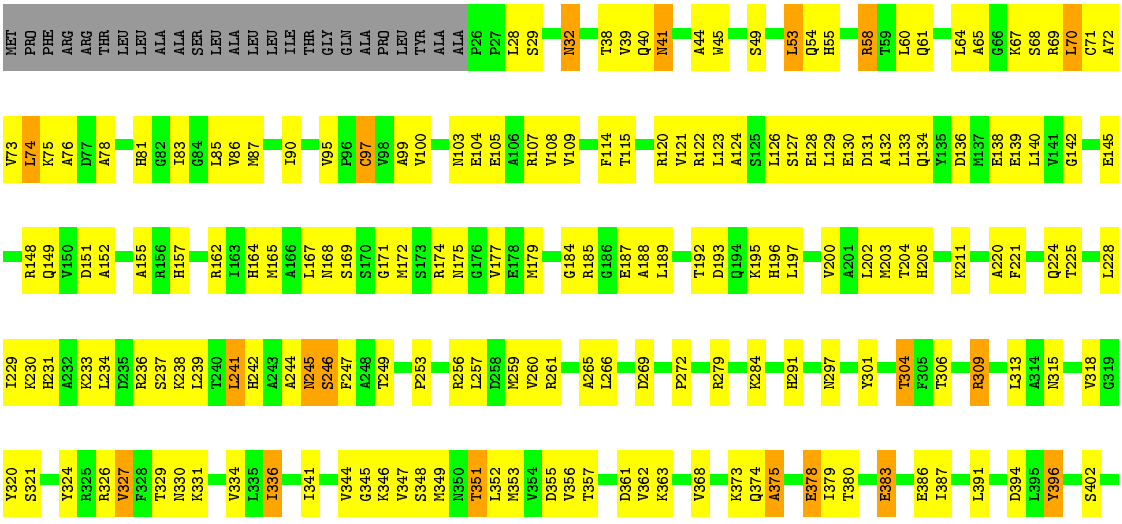
- Molecule 1: Broad specificity amino acid racemase

Chain A:



- Molecule 1: Broad specificity amino acid racemase

Chain B:




L407
V408
D409

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	142.42Å 118.11Å 74.02Å 90.00° 99.87° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 19.98 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-3.10) 98.9 (19.98-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.80 (at 3.09Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.175 , 0.219 0.182 , 0.190	Depositor DCC
R_{free} test set	1114 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å^2)	49.3	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5985	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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: PE1

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	0.81	2/2968 (0.1%)	0.70	0/4019
1	B	0.77	1/2968 (0.0%)	0.66	1/4019 (0.0%)
All	All	0.79	3/5936 (0.1%)	0.68	1/8038 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	223	GLU	CG-CD	5.55	1.60	1.51
1	B	58	ARG	CG-CD	5.27	1.65	1.51
1	A	97	CYS	CB-SG	-5.06	1.73	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	58	ARG	NE-CZ-NH1	5.04	122.82	120.30

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	2920	0	2914	164	0
1	B	2920	0	2914	148	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	25	0	21	9	0
2	B	25	0	21	12	0
3	A	48	0	0	11	0
3	B	47	0	0	9	0
All	All	5985	0	5870	297	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 25.

All (297) 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:174:ARG:HA	1:B:353:MET:HE2	1.15	1.13
1:A:69:ARG:HH12	1:A:240:THR:HG21	1.16	1.06
1:A:301:TYR:OH	2:B:501:PE1:HA	1.63	0.97
1:B:330:ASN:HD21	1:B:345:GLY:H	1.05	0.94
1:A:28:LEU:HD23	1:B:108:VAL:HG21	1.53	0.91
1:A:330:ASN:HD21	1:A:345:GLY:H	1.14	0.89
1:A:269:ASP:O	1:A:269:ASP:OD1	1.91	0.88
1:B:70:LEU:HD23	1:B:95:VAL:HG13	1.56	0.88
1:A:75:LYS:NZ	2:A:501:PE1:H	1.70	0.88
1:B:329:THR:HG23	1:B:346:LYS:HA	1.57	0.85
1:A:82:GLY:O	1:A:86:VAL:HG23	1.77	0.85
1:B:330:ASN:ND2	1:B:345:GLY:H	1.76	0.84
1:A:330:ASN:ND2	1:A:345:GLY:H	1.75	0.84
1:A:32:ASN:HD21	1:A:107:ARG:HH12	1.23	0.82
1:A:32:ASN:ND2	1:A:107:ARG:HH12	1.78	0.82
1:B:279:ARG:NH2	1:B:373:LYS:HE2	1.96	0.81
3:A:641:HOH:O	1:B:122:ARG:HB3	1.81	0.80
1:B:279:ARG:HH22	1:B:373:LYS:HE2	1.45	0.80
1:A:54:GLN:OE1	1:A:89:SER:HB3	1.82	0.79
1:A:174:ARG:CA	1:B:353:MET:HE2	2.07	0.79
1:A:164:HIS:HD2	1:A:242:HIS:CE1	2.01	0.78
1:B:38:THR:H	1:B:41:ASN:HD21	1.33	0.77
1:A:38:THR:H	1:A:41:ASN:HD21	1.31	0.76
1:B:336:ILE:HD13	1:B:368:VAL:HG13	1.68	0.76
1:B:336:ILE:CG1	1:B:341:ILE:HD12	2.17	0.75
1:A:295:ALA:HA	1:A:309:ARG:O	1.87	0.75
1:A:269:ASP:OD1	1:A:269:ASP:C	2.25	0.75
1:B:164:HIS:CD2	1:B:242:HIS:HE1	2.03	0.75
1:A:229:ILE:HA	1:A:234:LEU:CD1	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:HD21	1:A:86:VAL:CG1	2.17	0.74
1:A:314:ALA:HB3	1:A:354:VAL:HG22	1.69	0.74
1:A:242:HIS:HD2	1:A:261:ARG:HE	1.34	0.73
1:A:315:ASN:HD22	1:B:123:LEU:HD12	1.53	0.73
1:A:75:LYS:HZ2	2:A:501:PE1:H	1.33	0.73
1:A:75:LYS:HZ1	2:A:501:PE1:C4A	2.01	0.73
1:A:211:LYS:HD3	1:A:251:GLU:HB3	1.71	0.73
1:B:164:HIS:CD2	1:B:242:HIS:CE1	2.76	0.73
1:A:53:LEU:HD21	1:A:86:VAL:HG13	1.72	0.72
1:B:229:ILE:HD11	1:B:239:LEU:HD12	1.71	0.72
1:A:335:LEU:HG	1:A:379:ILE:HD12	1.71	0.72
1:B:149:GLN:O	1:B:152:ALA:HB3	1.89	0.72
1:A:309:ARG:HE	1:A:357:THR:HG21	1.54	0.72
1:B:330:ASN:HD21	1:B:345:GLY:N	1.86	0.71
1:B:261:ARG:NH1	2:B:501:PE1:N1	2.38	0.71
1:B:195:LYS:HA	1:B:195:LYS:HE2	1.73	0.70
1:A:75:LYS:NZ	2:A:501:PE1:N	2.39	0.70
1:A:330:ASN:HD21	1:A:345:GLY:N	1.88	0.70
1:A:164:HIS:CD2	1:A:242:HIS:CE1	2.80	0.69
1:A:164:HIS:CD2	1:A:242:HIS:HE1	2.11	0.69
1:B:246:SER:HB2	2:B:501:PE1:O2P	1.93	0.69
1:B:309:ARG:HD3	3:B:620:HOH:O	1.92	0.69
1:B:242:HIS:HD2	1:B:261:ARG:HE	1.40	0.69
1:B:336:ILE:HG12	1:B:341:ILE:HD12	1.73	0.68
1:A:97:CYS:SG	1:A:98:VAL:N	2.67	0.68
1:A:89:SER:O	1:A:93:GLN:HG2	1.93	0.67
1:A:69:ARG:NH1	1:A:240:THR:HG21	2.01	0.66
1:B:164:HIS:HD2	1:B:242:HIS:CE1	2.14	0.66
1:A:381:GLN:HG3	1:A:392:LEU:HD22	1.78	0.66
1:B:172:MET:CE	1:B:174:ARG:HH11	2.09	0.66
1:A:309:ARG:CG	1:A:310:ASP:H	2.07	0.65
1:A:75:LYS:HZ1	2:A:501:PE1:C4	2.09	0.65
1:A:120:ARG:HD2	1:A:139:GLU:OE1	1.96	0.65
1:B:336:ILE:HG13	1:B:341:ILE:CD1	2.26	0.65
1:A:223:GLU:HG3	3:A:613:HOH:O	1.97	0.65
1:A:326:ARG:HB2	1:B:394:ASP:OD1	1.97	0.65
1:A:229:ILE:HA	1:A:234:LEU:HD11	1.78	0.64
1:A:229:ILE:HA	1:A:234:LEU:HD12	1.80	0.64
1:A:190:GLN:O	1:A:194:GLN:NE2	2.31	0.64
1:A:279:ARG:HD2	3:A:601:HOH:O	1.97	0.64
1:A:242:HIS:CD2	1:A:261:ARG:HE	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ALA:O	1:A:224:GLN:HG3	1.97	0.63
1:B:220:ALA:O	1:B:224:GLN:HG3	1.97	0.63
1:A:48:VAL:HG11	1:A:81:HIS:HB3	1.80	0.63
1:A:81:HIS:NE2	1:A:281:MET:HB2	2.12	0.63
1:A:309:ARG:NE	1:A:357:THR:HG21	2.13	0.63
2:A:501:PE1:HA	1:B:301:TYR:OH	1.98	0.63
1:A:203:MET:HE2	1:A:204:THR:CA	2.30	0.62
1:B:38:THR:H	1:B:41:ASN:ND2	1.97	0.62
1:A:32:ASN:HD21	1:A:107:ARG:NH1	1.96	0.62
1:A:41:ASN:HD22	1:A:41:ASN:C	2.02	0.62
1:B:327:VAL:CG1	1:B:387:ILE:HG22	2.30	0.62
1:A:309:ARG:HG2	1:A:310:ASP:N	2.16	0.61
1:A:309:ARG:CG	1:A:310:ASP:N	2.63	0.61
1:A:314:ALA:HB3	1:A:354:VAL:CG2	2.30	0.61
1:A:29:SER:HB2	1:B:107:ARG:NH2	2.16	0.61
1:A:50:ALA:HB2	1:A:407:LEU:HD13	1.83	0.61
1:B:229:ILE:CD1	1:B:239:LEU:HD12	2.30	0.60
1:A:42:SER:O	1:A:286:HIS:HE1	1.84	0.60
1:A:48:VAL:HG13	1:A:81:HIS:HD2	1.66	0.60
1:B:327:VAL:HG13	1:B:387:ILE:HG22	1.82	0.60
1:A:53:LEU:HG	3:A:636:HOH:O	2.02	0.60
1:B:242:HIS:CD2	1:B:261:ARG:HE	2.18	0.60
1:A:315:ASN:OD1	1:A:351:THR:HG23	2.02	0.59
1:B:221:PHE:O	1:B:225:THR:HG23	2.01	0.59
1:B:374:GLN:O	1:B:375:ALA:C	2.41	0.59
1:A:38:THR:N	1:A:41:ASN:HD21	1.97	0.59
1:A:357:THR:HG22	1:A:357:THR:O	2.02	0.59
1:B:336:ILE:HG13	1:B:341:ILE:HD12	1.83	0.59
1:A:309:ARG:HE	1:A:357:THR:CG2	2.15	0.58
1:A:335:LEU:HG	1:A:379:ILE:CD1	2.34	0.58
1:A:203:MET:HE2	1:A:204:THR:HA	1.86	0.58
1:A:341:ILE:HG23	1:A:355:ASP:O	2.03	0.58
1:B:71:CYS:HA	1:B:97:CYS:O	2.04	0.57
1:A:263:GLY:O	1:A:266:LEU:HB2	2.04	0.57
1:A:309:ARG:HH21	1:A:357:THR:HG22	1.70	0.57
1:A:279:ARG:CD	3:A:601:HOH:O	2.52	0.56
1:B:396:TYR:C	1:B:396:TYR:CD1	2.79	0.56
1:B:356:VAL:HG11	1:B:362:VAL:HG11	1.87	0.56
1:B:168:ASN:ND2	1:B:171:GLY:HA2	2.21	0.56
1:B:120:ARG:NH1	1:B:139:GLU:OE2	2.37	0.55
1:B:244:ALA:HB3	1:B:260:VAL:HG12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:THR:O	1:A:160:THR:HG22	2.06	0.55
1:B:231:HIS:CD2	3:B:621:HOH:O	2.59	0.55
1:B:40:GLN:HG2	3:B:633:HOH:O	2.05	0.55
1:A:54:GLN:O	1:A:58:ARG:HB2	2.07	0.55
1:A:187:GLU:HA	1:A:190:GLN:HE21	1.72	0.55
1:A:330:ASN:ND2	1:A:345:GLY:N	2.48	0.55
1:A:174:ARG:HA	1:B:353:MET:CE	2.11	0.54
1:B:225:THR:O	1:B:229:ILE:HG12	2.07	0.54
1:B:151:ASP:HA	1:B:197:LEU:HD21	1.88	0.54
1:A:178:GLU:OE1	1:B:297:ASN:ND2	2.26	0.54
1:A:309:ARG:HD3	3:A:621:HOH:O	2.07	0.54
1:B:130:GLU:OE2	1:B:157:HIS:HE1	1.90	0.54
1:B:75:LYS:NZ	2:B:501:PE1:H	2.05	0.54
1:B:347:VAL:HG22	1:B:352:LEU:HD12	1.90	0.54
1:A:50:ALA:O	1:A:54:GLN:HG2	2.08	0.54
1:A:53:LEU:HD21	1:A:86:VAL:HG12	1.90	0.54
1:A:311:SER:HB3	1:A:357:THR:OG1	2.08	0.53
1:B:131:ASP:O	1:B:134:GLN:HG2	2.08	0.53
1:B:380:THR:OG1	1:B:383:GLU:HB3	2.08	0.53
1:A:261:ARG:NH1	2:A:501:PE1:N1	2.53	0.53
1:A:48:VAL:HG13	1:A:81:HIS:CD2	2.43	0.53
1:B:169:SER:HB2	1:B:204:THR:HG21	1.89	0.53
1:B:380:THR:N	1:B:383:GLU:OE1	2.41	0.53
1:B:329:THR:CG2	1:B:346:LYS:HA	2.34	0.53
1:A:162:ARG:HG2	1:A:200:VAL:HG11	1.91	0.52
1:A:374:GLN:O	1:A:375:ALA:C	2.47	0.52
1:B:142:GLY:HA3	1:B:175:ASN:O	2.09	0.52
1:B:165:MET:HE3	1:B:188:ALA:HA	1.90	0.52
1:A:321:SER:HB3	1:A:349:MET:HG2	1.92	0.52
1:A:270:THR:O	1:A:271:VAL:C	2.47	0.52
1:B:138:GLU:HG2	1:B:162:ARG:HB2	1.92	0.52
1:A:77:ASP:O	1:A:78:ALA:HB3	2.10	0.51
1:B:75:LYS:NZ	2:B:501:PE1:N	2.59	0.51
1:B:246:SER:OG	1:B:265:ALA:HB2	2.10	0.51
1:A:38:THR:H	1:A:41:ASN:ND2	2.02	0.51
1:B:383:GLU:O	1:B:386:GLU:HB3	2.10	0.51
1:B:272:PRO:HD3	3:B:631:HOH:O	2.10	0.51
1:A:194:GLN:N	1:A:194:GLN:NE2	2.58	0.51
1:A:357:THR:CG2	1:A:357:THR:O	2.58	0.51
1:A:26:PRO:N	1:A:403:ASN:HA	2.26	0.50
1:B:409:ASP:C	3:B:640:HOH:O	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLU:OE1	1:A:164:HIS:HE1	1.95	0.50
1:B:75:LYS:HZ1	2:B:501:PE1:H	1.57	0.50
1:A:31:ASP:O	1:A:32:ASN:HB2	2.11	0.50
1:A:26:PRO:HG2	3:A:634:HOH:O	2.11	0.50
1:B:205:HIS:NE2	1:B:245:ASN:HB3	2.27	0.50
1:B:165:MET:HE1	1:B:188:ALA:HB1	1.92	0.50
1:A:326:ARG:NH1	1:A:347:VAL:O	2.45	0.50
1:B:129:LEU:C	1:B:129:LEU:HD23	2.31	0.50
1:A:42:SER:O	1:A:286:HIS:CE1	2.62	0.50
1:B:73:VAL:HA	1:B:99:ALA:HB3	1.93	0.49
1:B:253:PRO:HA	1:B:256:ARG:HE	1.77	0.49
1:B:165:MET:HE2	1:B:167:LEU:HD21	1.94	0.49
1:B:75:LYS:CE	2:B:501:PE1:H4A1	2.42	0.49
1:A:143:SER:HB2	1:B:291:HIS:CD2	2.47	0.49
1:A:189:LEU:O	1:A:192:THR:HG23	2.13	0.49
1:A:57:ILE:HG21	1:A:93:GLN:HG3	1.94	0.49
1:B:195:LYS:CA	1:B:195:LYS:HE2	2.39	0.49
1:B:336:ILE:CG1	1:B:341:ILE:CD1	2.88	0.48
1:A:194:GLN:H	1:A:194:GLN:HE21	1.61	0.48
1:B:179:MET:O	1:B:185:ARG:NE	2.40	0.48
1:B:320:TYR:HA	1:B:324:TYR:O	2.12	0.48
1:A:75:LYS:HZ1	2:A:501:PE1:C3	2.25	0.48
1:A:247:PHE:CE2	1:A:251:GLU:HG3	2.49	0.48
1:A:71:CYS:HA	1:A:97:CYS:O	2.14	0.48
1:B:55:HIS:ND1	1:B:58:ARG:NH2	2.62	0.48
1:A:41:ASN:ND2	1:A:41:ASN:C	2.66	0.48
1:A:297:ASN:HB2	1:A:307:LEU:HD12	1.95	0.48
1:B:107:ARG:HG3	3:B:646:HOH:O	2.14	0.48
1:A:236:ARG:HA	1:A:236:ARG:HD2	1.50	0.47
1:A:51:SER:HB3	1:A:409:ASP:HB2	1.96	0.47
1:B:347:VAL:HG22	1:B:352:LEU:CD1	2.44	0.47
1:B:229:ILE:HA	1:B:234:LEU:HB2	1.96	0.47
1:A:203:MET:HB2	1:A:203:MET:HE3	1.67	0.47
1:A:28:LEU:CD2	1:B:108:VAL:HG21	2.36	0.47
1:B:284:LYS:HA	1:B:368:VAL:O	2.14	0.47
1:B:75:LYS:O	1:B:76:ALA:HB3	2.14	0.47
1:A:142:GLY:HA3	1:A:175:ASN:O	2.14	0.47
1:A:291:HIS:CE1	1:B:123:LEU:HD11	2.49	0.47
1:B:145:GLU:O	1:B:149:GLN:HG3	2.15	0.47
1:B:105:GLU:O	1:B:109:VAL:HG23	2.15	0.47
1:A:293:TYR:HA	1:A:294:PRO:HD3	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ASN:HD22	1:A:42:SER:N	2.13	0.47
1:A:69:ARG:HG2	1:A:96:PRO:HG3	1.97	0.47
1:A:242:HIS:HD2	1:A:261:ARG:NE	2.08	0.47
1:B:330:ASN:ND2	1:B:345:GLY:N	2.53	0.47
1:A:321:SER:HB3	1:A:349:MET:O	2.15	0.46
1:A:69:ARG:HH12	1:A:240:THR:CG2	2.05	0.46
1:A:301:TYR:HH	2:B:501:PE1:HA	1.74	0.46
2:B:501:PE1:H4A2	2:B:501:PE1:HB1C	1.61	0.46
1:B:78:ALA:O	1:B:81:HIS:N	2.39	0.46
1:A:388:ASN:CG	1:A:395:LEU:HD11	2.36	0.46
1:B:196:HIS:O	1:B:197:LEU:HD23	2.14	0.46
1:A:319:GLY:H	1:A:322:ASP:HB2	1.80	0.46
1:A:50:ALA:HB2	1:A:407:LEU:CD1	2.45	0.46
1:B:75:LYS:NZ	2:B:501:PE1:C4A	2.79	0.46
1:A:204:THR:O	1:A:261:ARG:NH2	2.48	0.46
1:A:290:VAL:HG13	1:A:313:LEU:O	2.16	0.45
1:B:269:ASP:C	1:B:269:ASP:OD1	2.54	0.45
1:B:100:VAL:HB	1:B:105:GLU:HB3	1.97	0.45
1:A:60:LEU:HD23	1:A:277:TYR:OH	2.16	0.45
1:A:87:MET:O	1:A:91:ILE:HG13	2.17	0.45
1:B:39:VAL:HG22	1:B:45:TRP:CE2	2.52	0.45
1:A:316:ILE:HG12	1:A:368:VAL:HG21	1.99	0.45
1:A:211:LYS:HD2	1:A:252:VAL:HG22	1.99	0.45
1:A:279:ARG:HH22	1:A:373:LYS:HG3	1.81	0.45
3:A:640:HOH:O	1:B:126:LEU:HG	2.17	0.45
1:B:32:ASN:HD22	1:B:32:ASN:N	2.15	0.45
1:B:104:GLU:O	1:B:108:VAL:HG23	2.17	0.45
1:B:172:MET:HE2	1:B:174:ARG:HH11	1.81	0.44
1:B:261:ARG:HB3	2:B:501:PE1:H6	2.00	0.44
1:A:178:GLU:OE2	1:A:180:ALA:HB2	2.17	0.44
1:B:247:PHE:C	1:B:247:PHE:CD1	2.90	0.44
1:B:355:ASP:OD1	1:B:357:THR:OG1	2.25	0.44
1:B:103:ASN:OD1	1:B:132:ALA:HB2	2.18	0.44
1:B:329:THR:HG23	1:B:346:LYS:CA	2.39	0.44
1:B:41:ASN:HD22	1:B:41:ASN:C	2.21	0.44
1:B:87:MET:CE	1:B:114:PHE:HB2	2.48	0.44
1:B:362:VAL:HB	3:B:617:HOH:O	2.17	0.44
1:A:121:VAL:HB	2:A:501:PE1:H2A3	2.00	0.44
1:A:104:GLU:O	1:A:108:VAL:HG23	2.18	0.44
1:B:202:LEU:HD12	1:B:241:LEU:HD11	2.00	0.44
1:A:315:ASN:ND2	1:B:123:LEU:HB2	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:ALA:O	1:B:155:ALA:HB3	2.17	0.43
1:B:279:ARG:HG3	3:B:602:HOH:O	2.18	0.43
1:B:321:SER:HB3	1:B:349:MET:HG2	1.98	0.43
1:B:65:ALA:HB3	1:B:67:LYS:HE2	2.00	0.43
1:A:238:LYS:HB3	1:A:238:LYS:HE2	1.67	0.43
3:A:641:HOH:O	1:B:122:ARG:CB	2.52	0.43
1:B:249:THR:OG1	1:B:260:VAL:HG11	2.18	0.43
1:A:362:VAL:C	1:A:363:LYS:HG2	2.38	0.43
1:B:72:ALA:HB1	1:B:74:LEU:HD13	2.01	0.43
1:A:151:ASP:HB2	1:A:194:GLN:HG3	1.99	0.43
1:A:140:LEU:HD11	1:A:166:ALA:HB2	1.99	0.43
1:A:312:ARG:N	1:A:357:THR:OG1	2.48	0.43
1:B:53:LEU:HD21	1:B:86:VAL:HG22	1.99	0.43
1:B:245:ASN:HA	1:B:261:ARG:O	2.19	0.43
1:A:205:HIS:HE1	1:B:301:TYR:OH	2.02	0.43
1:A:54:GLN:HB3	1:A:93:GLN:NE2	2.34	0.43
1:A:32:ASN:ND2	1:B:29:SER:OG	2.49	0.43
1:A:326:ARG:NH2	3:A:624:HOH:O	2.44	0.42
1:A:218:LEU:HG	1:A:222:ASN:HD21	1.84	0.42
1:A:37:LEU:HD22	1:A:404:PRO:HG3	2.01	0.42
1:A:355:ASP:OD1	1:A:357:THR:HB	2.20	0.42
1:B:373:LYS:HG2	1:B:378:GLU:HB2	2.01	0.42
1:B:331:LYS:HZ3	1:B:331:LYS:HG3	1.74	0.42
1:B:321:SER:HB3	1:B:349:MET:CG	2.49	0.42
1:B:140:LEU:HD11	1:B:203:MET:SD	2.59	0.42
1:A:71:CYS:SG	1:A:259:MET:SD	3.18	0.42
1:B:49:SER:HA	1:B:408:VAL:HG23	2.02	0.42
1:A:356:VAL:HG11	1:A:362:VAL:HG11	2.02	0.42
1:B:259:MET:CG	1:B:260:VAL:N	2.83	0.42
1:B:54:GLN:NE2	3:B:607:HOH:O	2.53	0.42
1:A:240:THR:HG22	1:A:258:ASP:HB3	2.01	0.41
1:A:279:ARG:HH12	1:A:373:LYS:NZ	2.17	0.41
1:A:312:ARG:O	1:A:313:LEU:HD12	2.20	0.41
1:A:315:ASN:HD22	1:B:123:LEU:CD1	2.29	0.41
1:A:48:VAL:CG1	1:A:81:HIS:CD2	3.04	0.41
1:B:64:LEU:HD13	1:B:68:SER:O	2.19	0.41
1:B:165:MET:CE	1:B:188:ALA:HB1	2.50	0.41
1:A:79:TYR:CZ	1:A:263:GLY:HA3	2.56	0.41
1:A:339:HIS:CD2	1:A:359:PHE:CE1	3.09	0.41
1:A:108:VAL:HG21	1:B:28:LEU:HD12	2.01	0.41
1:A:225:THR:O	1:A:226:ASP:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:MET:CE	1:A:204:THR:CA	2.98	0.41
1:A:46:VAL:O	1:A:46:VAL:HG12	2.20	0.41
1:B:124:ALA:HB1	1:B:128:GLU:HG2	2.01	0.41
1:B:165:MET:HE2	1:B:167:LEU:CD2	2.51	0.41
1:B:165:MET:HE3	1:B:188:ALA:CB	2.50	0.41
1:B:379:ILE:HD13	1:B:379:ILE:HA	1.84	0.41
1:B:407:LEU:HD23	1:B:407:LEU:HA	1.75	0.41
1:B:60:LEU:HA	1:B:60:LEU:HD23	1.94	0.41
1:A:223:GLU:HB2	3:A:613:HOH:O	2.21	0.41
1:A:392:LEU:O	1:A:393:ALA:C	2.59	0.41
1:B:151:ASP:OD2	1:B:196:HIS:ND1	2.33	0.41
1:B:53:LEU:HA	1:B:53:LEU:HD12	1.98	0.41
1:A:203:MET:CE	1:A:203:MET:C	2.89	0.40
1:A:54:GLN:H	1:A:54:GLN:HG2	1.67	0.40
1:B:184:GLY:O	1:B:187:GLU:HB2	2.21	0.40
1:B:315:ASN:OD1	1:B:351:THR:CG2	2.69	0.40
1:B:75:LYS:NZ	2:B:501:PE1:H4A1	2.36	0.40
1:B:172:MET:HE2	1:B:174:ARG:NH1	2.36	0.40
1:A:151:ASP:OD2	1:A:196:HIS:HB2	2.22	0.40
1:B:44:ALA:O	1:B:45:TRP:HB3	2.21	0.40
1:B:38:THR:O	1:B:40:GLN:N	2.55	0.40
1:A:372:GLY:O	1:A:378:GLU:HA	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	382/409 (93%)	339 (89%)	37 (10%)	6 (2%)	9 37
1	B	382/409 (93%)	332 (87%)	44 (12%)	6 (2%)	9 37
All	All	764/818 (93%)	671 (88%)	81 (11%)	12 (2%)	9 37

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	375	ALA
1	B	375	ALA
1	A	94	GLY
1	A	357	THR
1	B	304	THR
1	B	61	GLN
1	B	257	LEU
1	A	246	SER
1	A	366	ASN
1	B	230	LYS
1	B	245	ASN
1	A	271	VAL

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	307/325 (94%)	259 (84%)	48 (16%)	2 11
1	B	307/325 (94%)	257 (84%)	50 (16%)	2 10
All	All	614/650 (94%)	516 (84%)	98 (16%)	2 11

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	SER
1	A	32	ASN
1	A	41	ASN
1	A	46	VAL
1	A	48	VAL
1	A	53	LEU
1	A	54	GLN
1	A	68	SER
1	A	74	LEU
1	A	86	VAL
1	A	110	ARG

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Mol	Chain	Res	Type
1	A	115	THR
1	A	134	GLN
1	A	136	ASP
1	A	138	GLU
1	A	160	THR
1	A	177	VAL
1	A	183	SER
1	A	185	ARG
1	A	192	THR
1	A	194	GLN
1	A	195	LYS
1	A	198	LYS
1	A	202	LEU
1	A	203	MET
1	A	215	ARG
1	A	224	GLN
1	A	229	ILE
1	A	234	LEU
1	A	236	ARG
1	A	237	SER
1	A	240	THR
1	A	261	ARG
1	A	262	THR
1	A	269	ASP
1	A	270	THR
1	A	309	ARG
1	A	318	VAL
1	A	321	SER
1	A	326	ARG
1	A	344	VAL
1	A	353	MET
1	A	379	ILE
1	A	395	LEU
1	A	398	VAL
1	A	405	LYS
1	A	407	LEU
1	A	409	ASP
1	B	32	ASN
1	B	41	ASN
1	B	53	LEU
1	B	69	ARG
1	B	70	LEU

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Mol	Chain	Res	Type
1	B	74	LEU
1	B	83	ILE
1	B	85	LEU
1	B	90	ILE
1	B	97	CYS
1	B	115	THR
1	B	121	VAL
1	B	127	SER
1	B	133	LEU
1	B	136	ASP
1	B	148	ARG
1	B	177	VAL
1	B	189	LEU
1	B	192	THR
1	B	193	ASP
1	B	200	VAL
1	B	211	LYS
1	B	228	LEU
1	B	233	LYS
1	B	236	ARG
1	B	237	SER
1	B	238	LYS
1	B	241	LEU
1	B	246	SER
1	B	266	LEU
1	B	304	THR
1	B	306	THR
1	B	309	ARG
1	B	313	LEU
1	B	318	VAL
1	B	326	ARG
1	B	327	VAL
1	B	334	VAL
1	B	336	ILE
1	B	344	VAL
1	B	348	SER
1	B	351	THR
1	B	361	ASP
1	B	363	LYS
1	B	378	GLU
1	B	383	GLU
1	B	391	LEU

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Mol	Chain	Res	Type
1	B	396	TYR
1	B	402	SER
1	B	407	LEU

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	32	ASN
1	A	41	ASN
1	A	164	HIS
1	A	194	GLN
1	A	205	HIS
1	A	222	ASN
1	A	242	HIS
1	A	286	HIS
1	A	291	HIS
1	A	315	ASN
1	A	330	ASN
1	A	339	HIS
1	A	350	ASN
1	B	32	ASN
1	B	41	ASN
1	B	43	ASN
1	B	54	GLN
1	B	157	HIS
1	B	164	HIS
1	B	222	ASN
1	B	242	HIS
1	B	291	HIS
1	B	330	ASN
1	B	339	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)

2 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	PE1	B	501	-	22,25,25	1.18	2 (9%)	26,34,34	1.46	4 (15%)
2	PE1	A	501	-	22,25,25	1.06	1 (4%)	26,34,34	1.49	6 (23%)

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	PE1	B	501	-	-	11/16/20/20	0/1/1/1
2	PE1	A	501	-	-	9/16/20/20	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	PE1	CB-CA	3.16	1.57	1.53
2	A	501	PE1	C4A-C4	2.94	1.55	1.51
2	B	501	PE1	C3-C4	2.34	1.43	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	PE1	C4A-C4-C3	3.87	124.19	120.04
2	B	501	PE1	C4A-N-CA	3.53	120.61	113.83
2	B	501	PE1	C4A-C4-C3	3.13	123.39	120.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	PE1	C4A-N-CA	2.72	119.06	113.83
2	B	501	PE1	O4P-C5A-C5	2.59	114.28	109.35
2	B	501	PE1	C4A-C4-C5	-2.51	116.92	119.71
2	A	501	PE1	C4-C4A-N	2.40	118.40	111.78
2	A	501	PE1	O3P-P-O2P	2.24	116.20	107.64
2	A	501	PE1	O3P-P-O4P	-2.18	100.93	106.73
2	A	501	PE1	C4A-C4-C5	-2.02	117.46	119.71

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	PE1	C5-C4-C4A-N
2	B	501	PE1	CB-CA-N-C4A
2	B	501	PE1	C-CA-CB-CG
2	A	501	PE1	C5-C4-C4A-N
2	A	501	PE1	C-CA-CB-CG
2	A	501	PE1	N-CA-CB-CG
2	A	501	PE1	C4-C4A-N-CA
2	B	501	PE1	N-CA-CB-CG
2	B	501	PE1	C4-C4A-N-CA
2	B	501	PE1	CE-CD-CG-CB
2	A	501	PE1	CE-CD-CG-CB
2	B	501	PE1	C3-C4-C4A-N
2	B	501	PE1	C-CA-N-C4A
2	B	501	PE1	CA-CB-CG-CD
2	B	501	PE1	CG-CD-CE-NZ
2	B	501	PE1	C5A-O4P-P-O1P
2	A	501	PE1	CG-CD-CE-NZ
2	A	501	PE1	C-CA-N-C4A
2	A	501	PE1	C3-C4-C4A-N
2	A	501	PE1	CB-CA-N-C4A

There are no ring outliers.

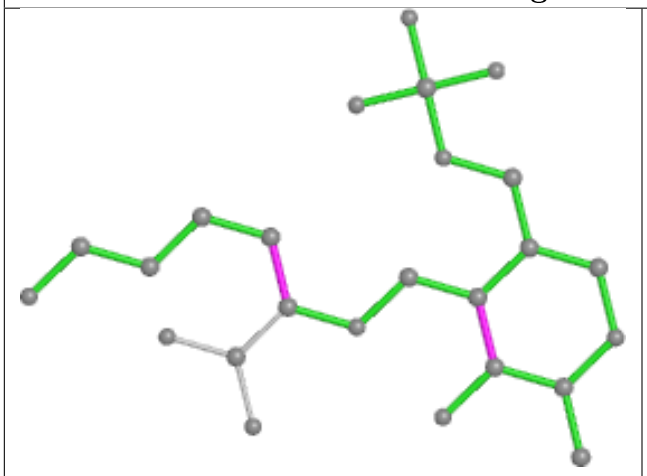
2 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	PE1	12	0
2	A	501	PE1	9	0

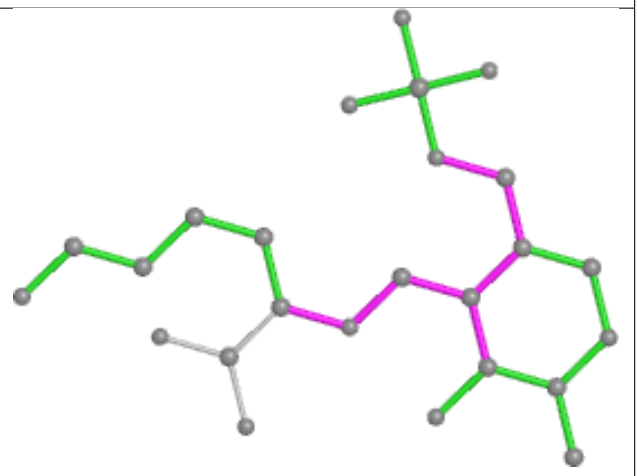
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

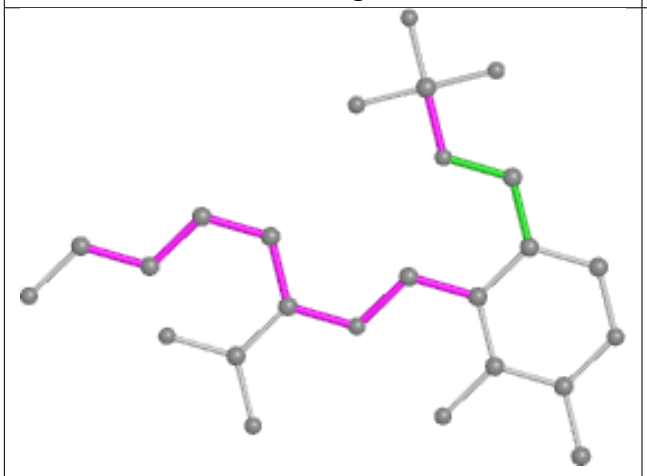
Ligand PE1 B 501



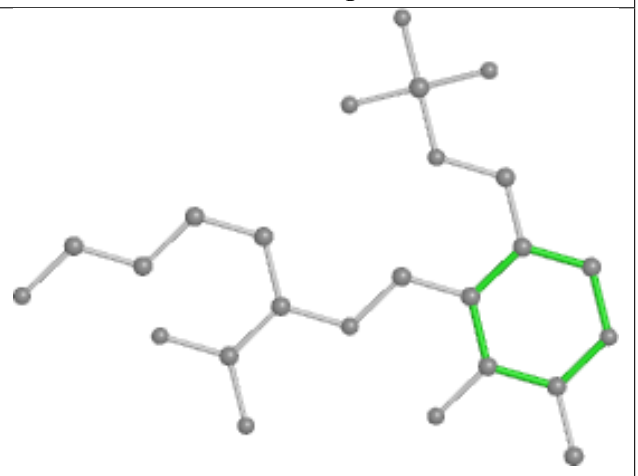
Bond lengths



Bond angles

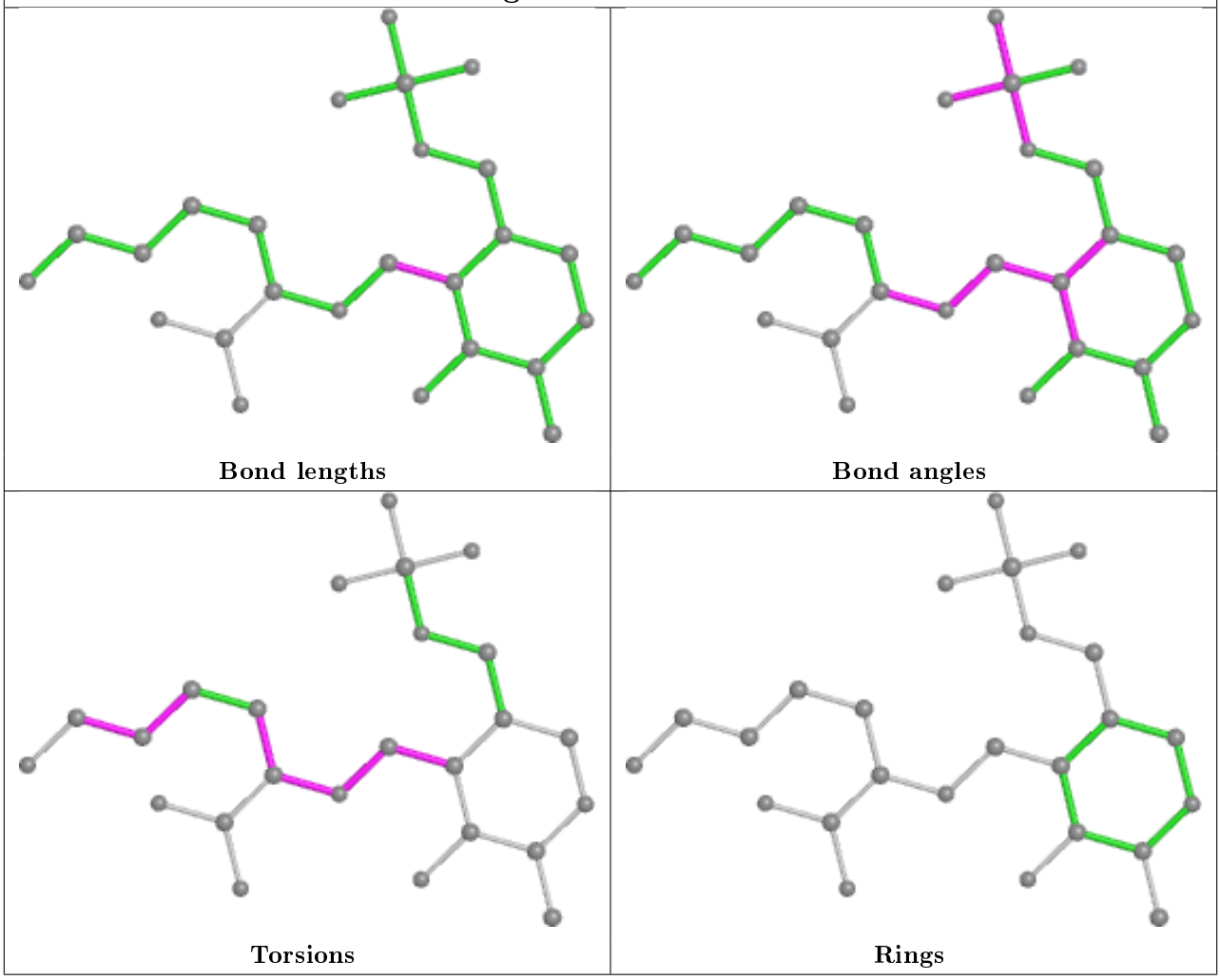


Torsions



Rings

Ligand PE1 A 501



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	384/409 (93%)	-0.76	0	100	100	29, 42, 54, 67	0
1	B	384/409 (93%)	-0.78	0	100	100	31, 43, 56, 67	0
All	All	768/818 (93%)	-0.77	0	100	100	29, 42, 55, 67	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

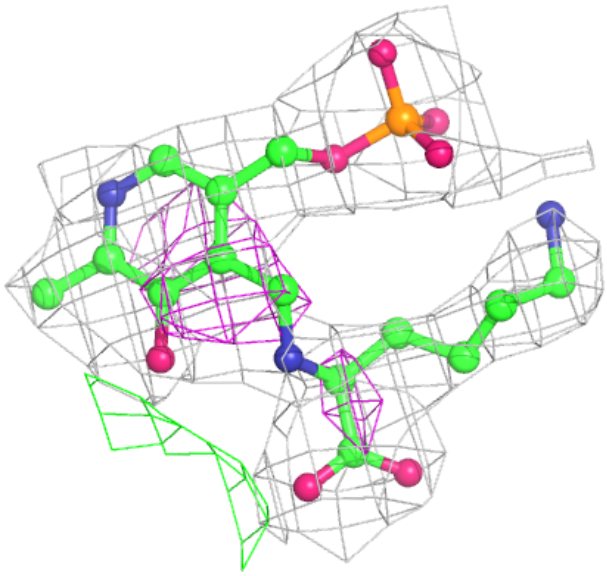
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

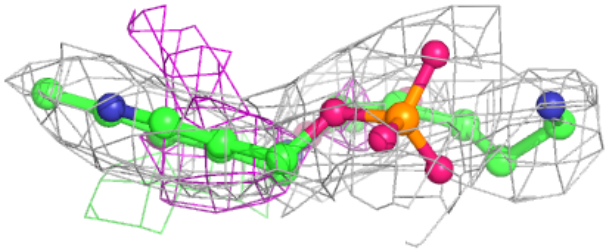
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PE1	B	501	25/25	0.91	0.21	42,48,52,53	0
2	PE1	A	501	25/25	0.93	0.20	52,59,64,64	0

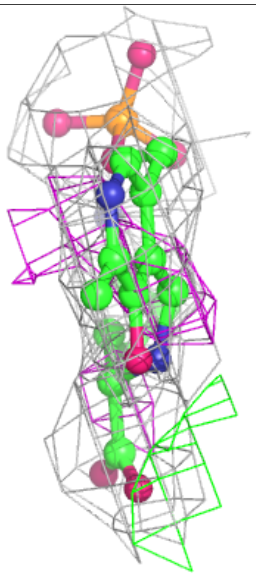
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PE1 B 501:

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

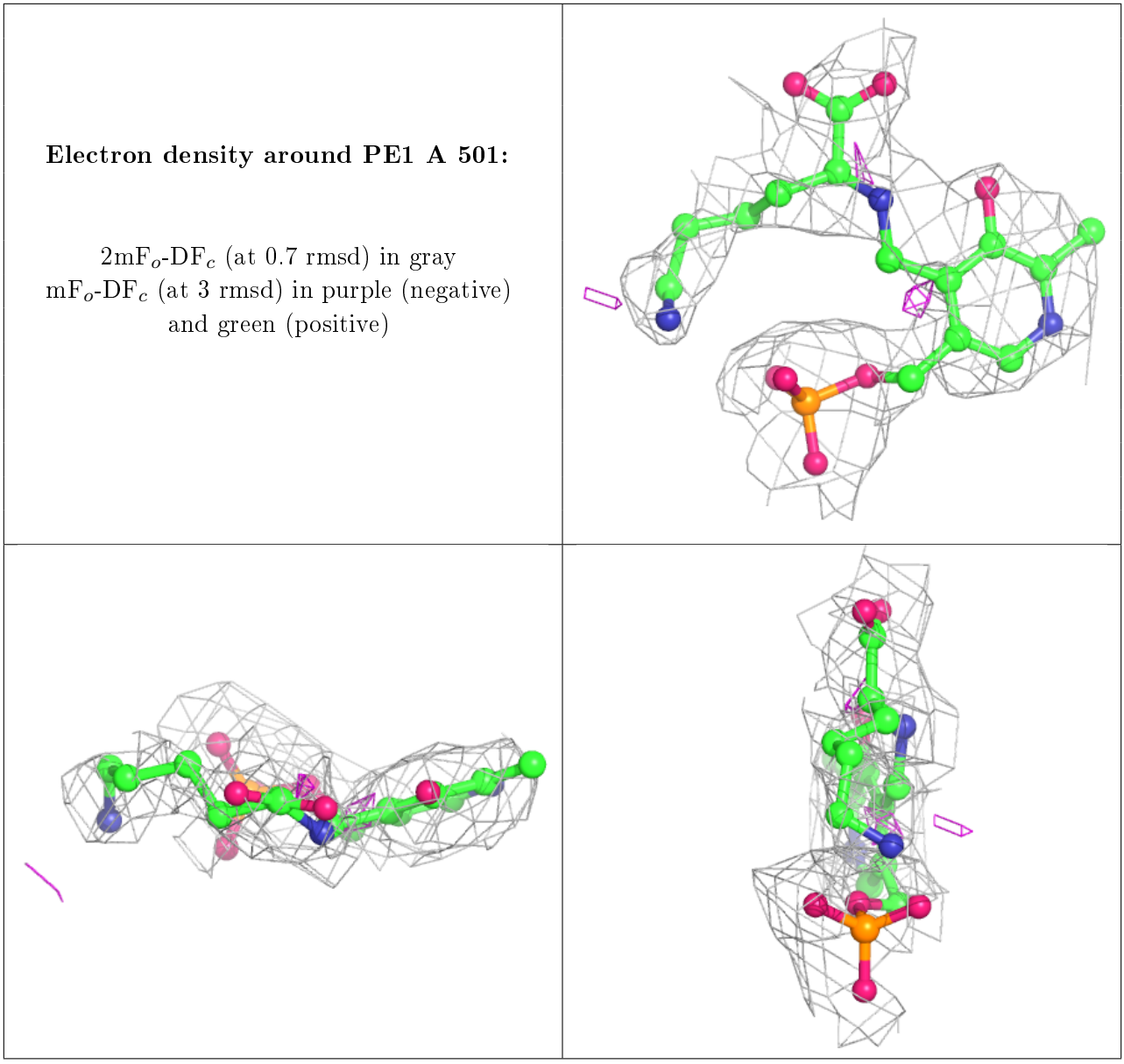






Electron density around PE1 A 501:

$2mF_o$-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

There are no such residues in this entry.