Full wwPDB X-ray Structure Validation Report (i)

Jun 19, 2024 – 09:01 AM EDT

PDB ID	:	4MRV
Title	:	Structure of a bacterial Atm1-family ABC transporter
Authors	:	Lee, J.Y.; Yang, J.G.; Zhitnitsky, D.; Lewinson, O.; Rees, D.C.
Deposited on	:	2013-09-17
Resolution	:	2.50 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 (i) 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 (i)) were used in the production of this report:

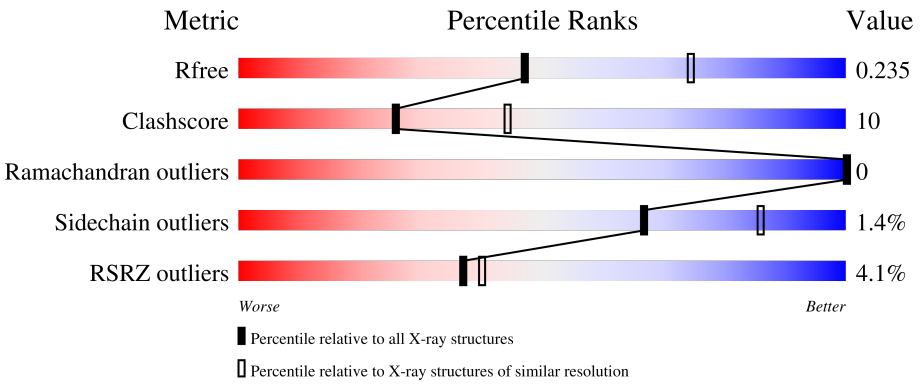
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	614	4% 78% 20% •
1	B	614	4% 76% 21% •

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	HGD	A	701	-	-	-	X
4	PO4	A	705	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9734 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

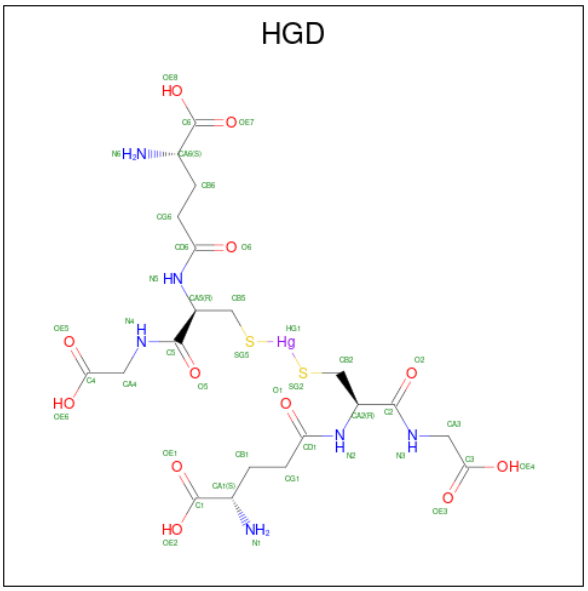
- Molecule 1 is a protein called ABC transporter related protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	600	4658	2970	828	848	12	0	0	0
1	B	598	4645	2963	825	845	12	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

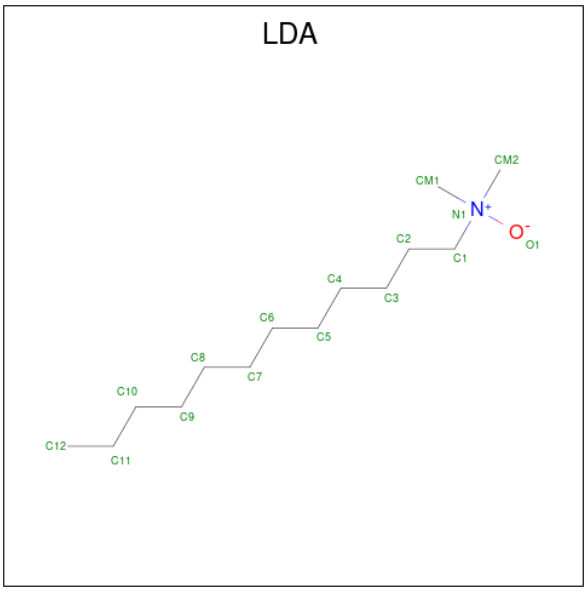
Chain	Residue	Modelled	Actual	Comment	Reference
A	609	HIS	-	EXPRESSION TAG	UNP Q2G506
A	610	HIS	-	EXPRESSION TAG	UNP Q2G506
A	611	HIS	-	EXPRESSION TAG	UNP Q2G506
A	612	HIS	-	EXPRESSION TAG	UNP Q2G506
A	613	HIS	-	EXPRESSION TAG	UNP Q2G506
A	614	HIS	-	EXPRESSION TAG	UNP Q2G506
B	609	HIS	-	EXPRESSION TAG	UNP Q2G506
B	610	HIS	-	EXPRESSION TAG	UNP Q2G506
B	611	HIS	-	EXPRESSION TAG	UNP Q2G506
B	612	HIS	-	EXPRESSION TAG	UNP Q2G506
B	613	HIS	-	EXPRESSION TAG	UNP Q2G506
B	614	HIS	-	EXPRESSION TAG	UNP Q2G506

- Molecule 2 is mercury bis(L-gamma-glutamyl-3-sulfido-L-alanylglycine) (three-letter code: HGD) (formula: $C_{20}H_{32}HgN_6O_{12}S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Hg	N	O	S		
2	A	1	41	20	1	6	12	2	0	0

- Molecule 3 is LAURYL DIMETHYLAMINE-N-OXIDE (three-letter code: LDA) (formula: $C_{14}H_{31}NO$).



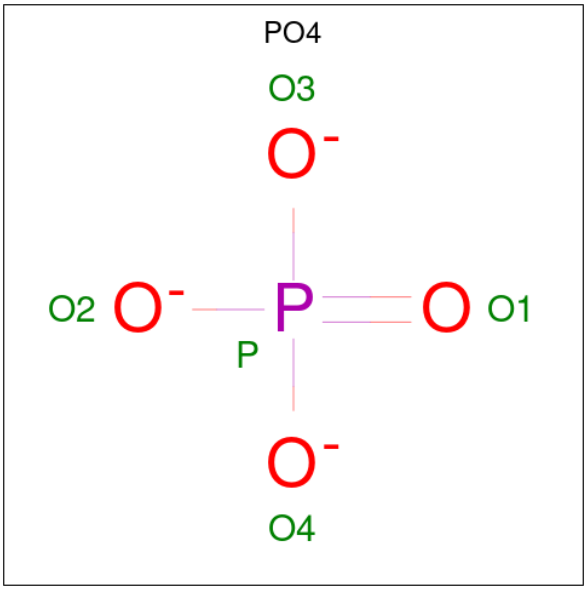
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	16	14	1	1	0	0
3	A	1	16	14	1	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	B	1	16	14	1	1	0	0
			Total	C	N	O		
3	B	1	16	14	1	1	0	0

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



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

- Molecule 5 is water.

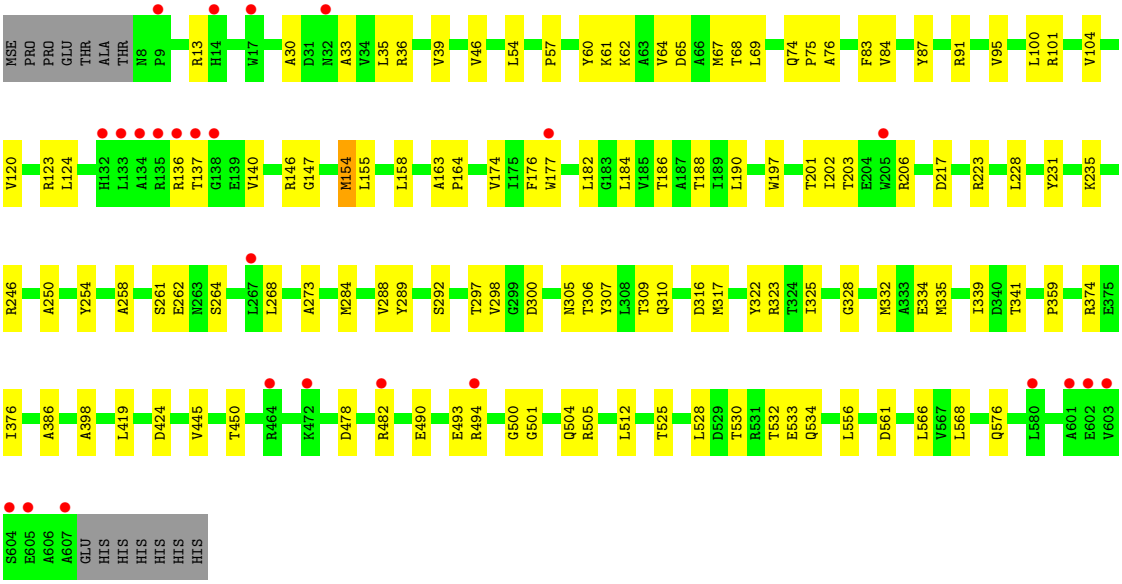
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	149	149	149	0	0
			Total	O		
5	B	157	157	157	0	0

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.

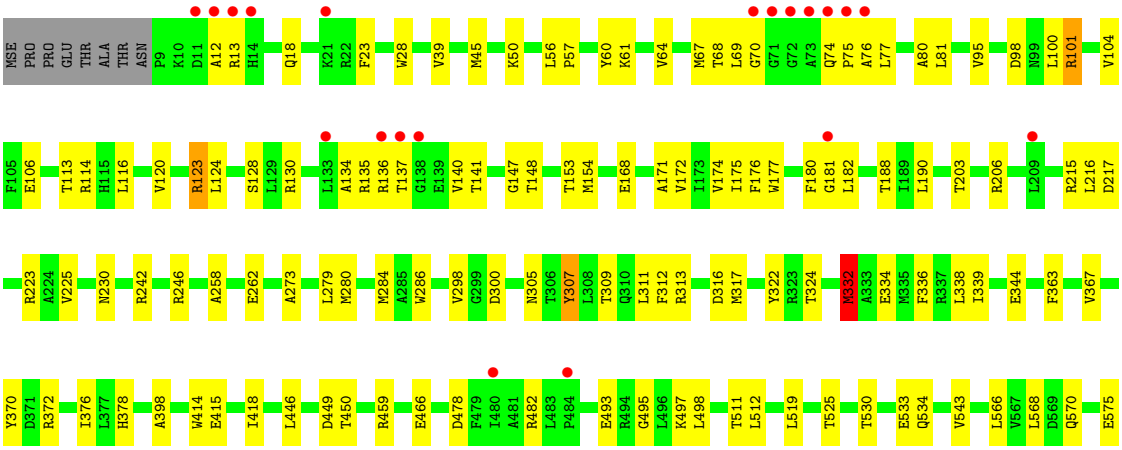
• Molecule 1: ABC transporter related protein

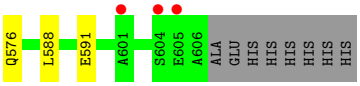
Chain A:



• Molecule 1: ABC transporter related protein

Chain B:




Q576
L588
E591
A601
S604
E605
A606
ALA
GLU
HIS
HIS
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Sourc
Space group	C 1 2 1	Deposi
Cell constants a, b, c, α, β, γ	322.44Å 95.62Å 78.91Å 90.00° 101.52° 90.00°	Deposi
Resolution (Å)	39.49 – 2.50 39.49 – 2.50	Deposi EDS
% Data completeness (in resolution range)	98.3 (39.49-2.50) 84.4 (39.49-2.50)	Deposi EDS
R_{merge}	(Not available)	Deposi
R_{sym}	(Not available)	Deposi
$< I/\sigma(I) >$ [1]	0.41 (at 2.51Å)	Xtriag
Refinement program	PHENIX (phenix.refine: 1.8.2_1309), REFMAC (rigid body)	Deposi
R, R_{free}	0.206 , 0.234 0.209 , 0.235	Deposi DCC
R_{free} test set	4014 reflections (4.99%)	wwPDB
Wilson B-factor (Å^2)	52.5	Xtriag
Anisotropy	0.376	Xtriag
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 49.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriag
Estimated twinning fraction	0.026 for -h-2*l,-k,l	Xtriag
F_o,F_c correlation	0.95	EDS
Total number of atoms	9734	wwPDB
Average B, all atoms (Å^2)	60.0	wwPDB

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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 (i)

5.1 Standard geometry (i)

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

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	0.47	0/4732	0.64	0/6408
1	B	0.47	0/4719	0.66	1/6389 (0.0%)
All	All	0.47	0/9451	0.65	1/12797 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	332	MSE	CG-SE-CE	-5.28	87.30	98.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4658	0	4733	108	1
1	B	4645	0	4723	103	1
2	A	41	0	29	9	0
3	A	32	0	62	8	0
3	B	32	0	62	6	0
4	A	10	0	0	1	0
4	B	10	0	0	1	0
5	A	149	0	0	11	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	157	0	0	10	1
All	All	9734	0	9609	199	2

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 10.

All (199) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:ILE:O	5:B:839:HOH:O	1.81	0.99
1:A:64:VAL:HA	1:A:67:MSE:HE2	1.51	0.92
1:A:146:ARG:NH1	5:A:948:HOH:O	2.03	0.90
1:B:61:LYS:NZ	1:B:300:ASP:OD1	2.07	0.88
1:A:494:ARG:HG3	1:B:136:ARG:HH22	1.47	0.79
1:A:374:ARG:NH1	5:A:922:HOH:O	2.15	0.78
1:B:215:ARG:NH2	5:B:877:HOH:O	2.15	0.77
1:A:317:MSE:HG2	2:A:701:HGD:H25	1.66	0.77
1:A:61:LYS:NZ	1:A:300:ASP:OD1	2.19	0.75
1:B:68:THR:HG21	1:B:298:VAL:HG11	1.68	0.74
1:B:128:SER:OG	5:B:924:HOH:O	2.07	0.73
1:A:67:MSE:HE3	1:B:298:VAL:HG23	1.71	0.72
1:A:424:ASP:OD2	5:A:817:HOH:O	2.07	0.72
1:A:136:ARG:NH2	1:B:493:GLU:OE1	2.23	0.71
1:B:284:MSE:HE3	1:B:305:ASN:HB2	1.70	0.71
1:B:130:ARG:NH2	1:B:370:TYR:O	2.23	0.70
1:A:123:ARG:NH2	1:A:341:THR:O	2.24	0.70
1:B:206:ARG:NH2	4:B:704:PO4:O4	2.24	0.70
1:B:180:PHE:O	5:B:925:HOH:O	2.09	0.70
1:A:334:GLU:HG2	3:A:702:LDA:H12	1.74	0.69
1:B:23:PHE:CD1	1:B:332:MSE:HE1	2.28	0.69
1:A:223:ARG:NE	5:A:913:HOH:O	2.25	0.69
1:B:566:LEU:HD23	1:B:576:GLN:HG3	1.75	0.68
1:B:223:ARG:HD3	1:B:246:ARG:HG2	1.75	0.68
1:A:566:LEU:HD23	1:A:576:GLN:HG3	1.74	0.67
1:B:50:LYS:NZ	1:B:168:GLU:OE2	2.27	0.66
1:A:525:THR:HB	1:A:533:GLU:HG3	1.76	0.66
1:A:101:ARG:NH2	5:A:909:HOH:O	1.99	0.66
1:A:316:ASP:O	2:A:701:HGD:N6	2.30	0.65
1:A:323:ARG:NH2	4:A:705:PO4:O3	2.29	0.65
1:B:575:GLU:OE1	1:B:588:LEU:N	2.29	0.65
1:A:223:ARG:NH1	5:A:910:HOH:O	2.29	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ARG:NH1	1:A:261:SER:O	2.30	0.64
1:B:74:GLN:HB3	1:B:75:PRO:HD2	1.79	0.62
1:B:147:GLY:HA3	3:B:702:LDA:H32	1.81	0.62
1:B:493:GLU:HA	1:B:495:GLY:N	2.14	0.62
1:A:147:GLY:HA3	3:A:702:LDA:H41	1.81	0.62
1:B:45:MSE:HE3	1:B:100:LEU:HB3	1.82	0.61
1:A:146:ARG:HH22	3:A:702:LDA:HM22	1.66	0.61
1:B:398:ALA:HB1	1:B:568:LEU:HB2	1.83	0.60
1:A:398:ALA:HB1	1:A:568:LEU:HB2	1.84	0.60
1:A:501:GLY:O	1:A:505:ARG:HG3	2.00	0.60
1:A:177:TRP:CZ3	1:A:182:LEU:HD22	2.37	0.60
1:B:446:LEU:O	5:B:846:HOH:O	2.17	0.59
1:A:64:VAL:HA	1:A:67:MSE:CE	2.31	0.59
1:A:223:ARG:NH1	1:A:250:ALA:HB2	2.18	0.58
1:A:68:THR:HG21	1:A:298:VAL:HG11	1.85	0.58
1:B:98:ASP:O	1:B:101:ARG:HG2	2.03	0.58
1:A:530:THR:O	1:A:534:GLN:HG2	2.03	0.58
1:B:148:THR:HG23	3:B:702:LDA:H112	1.85	0.58
1:B:511:THR:HG21	1:B:519:LEU:HD13	1.86	0.58
1:B:116:LEU:HD22	1:B:332:MSE:HE3	1.85	0.58
1:B:334:GLU:HG2	3:B:702:LDA:HM11	1.85	0.57
1:B:493:GLU:HA	1:B:495:GLY:H	1.68	0.57
1:A:146:ARG:NH2	3:A:702:LDA:HM22	2.20	0.56
1:A:359:PRO:HD2	1:A:386:ALA:HB1	1.88	0.56
1:A:297:THR:HG23	1:A:300:ASP:H	1.70	0.56
1:B:242:ARG:NH2	5:B:876:HOH:O	2.38	0.56
1:A:154:MSE:HB2	1:A:325:ILE:HA	1.88	0.55
1:B:114:ARG:NE	5:B:850:HOH:O	2.04	0.55
1:B:23:PHE:HB2	1:B:332:MSE:HE1	1.88	0.55
1:A:154:MSE:HG2	1:A:328:GLY:HA3	1.89	0.55
1:A:206:ARG:NH1	1:A:264:SER:OG	2.39	0.55
1:A:65:ASP:OD1	1:A:297:THR:OG1	2.18	0.54
1:B:130:ARG:HD2	1:B:344:GLU:OE1	2.06	0.54
1:B:313:ARG:NH2	5:B:838:HOH:O	2.14	0.54
1:B:124:LEU:HD21	1:B:338:LEU:HD13	1.90	0.54
3:A:702:LDA:H112	5:A:912:HOH:O	2.07	0.54
1:B:57:PRO:HG2	1:B:307:TYR:HE1	1.73	0.54
1:B:181:GLY:H	1:B:286:TRP:HH2	1.55	0.53
1:A:154:MSE:HE2	1:A:155:LEU:HA	1.91	0.53
1:A:246:ARG:NH1	5:A:928:HOH:O	2.41	0.53
1:A:136:ARG:O	1:A:140:VAL:HG23	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:LEU:HD11	1:B:498:LEU:HD12	1.89	0.53
1:A:284:MSE:HE3	1:A:305:ASN:HB2	1.89	0.53
1:B:512:LEU:HD21	1:B:543:VAL:HG13	1.90	0.52
1:A:231:TYR:OH	1:A:235:LYS:HE2	2.09	0.52
1:A:91:ARG:NH1	1:B:280:MSE:HE3	2.23	0.52
1:A:91:ARG:HH12	1:B:280:MSE:HE3	1.74	0.52
2:A:701:HGD:SG2	1:B:317:MSE:HG2	2.49	0.52
1:A:174:VAL:O	1:A:177:TRP:HB3	2.09	0.52
1:A:62:LYS:HB3	1:A:83:PHE:CE2	2.44	0.52
1:A:74:GLN:HA	1:A:75:PRO:C	2.30	0.51
1:A:155:LEU:HD11	1:A:332:MSE:HE1	1.92	0.51
1:A:262:GLU:HG3	1:B:106:GLU:OE2	2.11	0.51
1:B:172:VAL:HG22	1:B:307:TYR:CD2	2.45	0.51
1:B:258:ALA:O	1:B:262:GLU:HG2	2.11	0.51
1:B:13:ARG:NE	5:B:807:HOH:O	2.19	0.51
1:A:258:ALA:O	1:A:262:GLU:HG2	2.11	0.51
1:A:176:PHE:HE2	1:A:188:THR:HG21	1.76	0.50
1:B:372:ARG:HD2	1:B:414:TRP:CZ2	2.46	0.50
1:A:317:MSE:HE2	2:A:701:HGD:SG5	2.51	0.50
1:B:120:VAL:O	1:B:124:LEU:HG	2.12	0.49
1:A:298:VAL:HG23	1:B:67:MSE:HE2	1.94	0.49
1:A:95:VAL:HG11	1:B:273:ALA:HB2	1.94	0.49
1:B:28:TRP:HZ3	1:B:39:VAL:HB	1.77	0.49
1:B:493:GLU:OE2	1:B:497:LYS:HE2	2.12	0.49
1:B:68:THR:C	1:B:70:GLY:HA3	2.33	0.49
1:A:292:SER:OG	1:B:77:LEU:HD13	2.13	0.49
1:B:174:VAL:O	1:B:177:TRP:HB3	2.13	0.48
1:B:182:LEU:HA	5:B:925:HOH:O	2.13	0.48
1:A:154:MSE:HE1	1:A:158:LEU:HD12	1.95	0.48
1:A:197:TRP:O	1:A:201:THR:HG23	2.12	0.48
1:B:305:ASN:O	1:B:309:THR:HG23	2.13	0.48
1:A:317:MSE:HE1	2:A:701:HGD:H16	1.96	0.48
1:A:445:VAL:HG11	1:B:230:ASN:OD1	2.14	0.48
1:B:56:LEU:HD12	1:B:57:PRO:HD3	1.94	0.48
1:A:67:MSE:CE	1:B:298:VAL:HG23	2.41	0.48
1:B:56:LEU:N	1:B:57:PRO:HD2	2.29	0.48
1:B:64:VAL:HG12	1:B:298:VAL:HG13	1.96	0.48
1:A:123:ARG:HD2	1:A:123:ARG:HA	1.55	0.47
1:A:223:ARG:CZ	5:A:910:HOH:O	2.62	0.47
1:B:153:THR:HG22	1:B:324:THR:HG21	1.97	0.47
1:B:188:THR:HG22	1:B:279:LEU:HD11	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:MSE:HE2	1:B:336:PHE:CE2	2.49	0.47
1:B:134:ALA:O	1:B:135:ARG:HG3	2.14	0.47
1:B:74:GLN:C	1:B:76:ALA:H	2.17	0.46
1:B:177:TRP:CZ3	1:B:182:LEU:HD22	2.50	0.46
1:B:23:PHE:CG	1:B:332:MSE:HE1	2.50	0.46
1:A:203:THR:HG21	1:A:322:TYR:HD2	1.78	0.46
1:A:176:PHE:CE2	1:A:188:THR:HG21	2.51	0.46
1:B:113:THR:HB	3:B:702:LDA:H111	1.96	0.46
1:A:289:TYR:O	1:A:292:SER:HB2	2.16	0.46
1:B:530:THR:O	1:B:534:GLN:HG2	2.16	0.46
1:A:62:LYS:HB3	1:A:83:PHE:CD2	2.51	0.45
1:B:176:PHE:HE2	1:B:188:THR:HG21	1.80	0.45
1:A:273:ALA:HB2	1:B:95:VAL:HG11	1.97	0.45
1:A:525:THR:CB	1:A:533:GLU:HG3	2.46	0.45
1:B:100:LEU:O	1:B:104:VAL:HG23	2.16	0.45
1:A:46:VAL:HA	1:A:101:ARG:HH11	1.82	0.45
1:A:528:LEU:HD13	1:A:532:THR:HG22	1.99	0.45
1:A:335:MSE:HE3	3:A:702:LDA:H51	1.99	0.45
1:B:123:ARG:HD2	1:B:339:ILE:HA	1.98	0.45
1:B:217:ASP:OD1	3:B:701:LDA:HM13	2.16	0.45
1:B:525:THR:HB	1:B:533:GLU:HG3	1.98	0.45
1:A:54:LEU:O	1:A:57:PRO:HD2	2.17	0.44
1:A:87:TYR:CZ	1:A:91:ARG:HD2	2.52	0.44
3:A:702:LDA:H112	5:A:914:HOH:O	2.18	0.44
1:B:334:GLU:HG2	3:B:702:LDA:H11	1.99	0.44
1:A:74:GLN:HA	1:A:76:ALA:N	2.33	0.44
1:B:12:ALA:HB3	1:B:18:GLN:NE2	2.33	0.44
1:B:203:THR:HG21	1:B:322:TYR:HD2	1.82	0.44
1:A:268:LEU:HD23	2:A:701:HGD:H26	1.98	0.44
1:B:367:VAL:HB	1:B:415:GLU:HB2	2.00	0.44
1:A:316:ASP:O	2:A:701:HGD:H33	2.17	0.44
1:A:297:THR:O	1:A:300:ASP:HB2	2.17	0.44
1:B:23:PHE:CB	1:B:332:MSE:HE1	2.48	0.44
1:A:61:LYS:HZ1	1:A:297:THR:CG2	2.31	0.43
1:A:306:THR:O	1:A:310:GLN:HG3	2.18	0.43
1:B:68:THR:O	1:B:69:LEU:HD23	2.18	0.43
1:B:378:HIS:HD2	1:B:570:GLN:O	2.01	0.43
1:B:363:PHE:CE1	1:B:418:ILE:HD12	2.54	0.43
1:A:61:LYS:HZ1	1:A:297:THR:HG21	1.82	0.43
1:A:101:ARG:NE	5:A:909:HOH:O	2.52	0.43
1:A:217:ASP:HB2	1:A:254:TYR:CE1	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:ASP:O	1:B:482:ARG:HG3	2.18	0.43
1:B:177:TRP:HZ3	1:B:182:LEU:HD22	1.83	0.43
1:A:478:ASP:O	1:A:482:ARG:HG3	2.18	0.43
1:B:216:LEU:HD23	1:B:216:LEU:HA	1.86	0.43
1:A:450:THR:HA	1:A:490:GLU:HA	2.01	0.43
1:B:136:ARG:O	1:B:140:VAL:HG23	2.19	0.43
1:A:184:LEU:O	1:A:188:THR:HG23	2.19	0.42
1:A:35:LEU:O	1:A:39:VAL:HG23	2.19	0.42
1:A:500:GLY:O	1:A:504:GLN:HG2	2.19	0.42
1:A:419:LEU:HD23	1:A:424:ASP:HA	2.00	0.42
2:A:701:HGD:N1	1:B:316:ASP:O	2.52	0.42
1:A:33:ALA:HA	1:A:36:ARG:CZ	2.50	0.42
1:A:493:GLU:O	1:A:494:ARG:HB2	2.19	0.42
1:A:137:THR:HG23	1:B:225:VAL:HG11	2.00	0.42
1:A:494:ARG:CG	1:B:136:ARG:HH12	2.32	0.42
2:A:701:HGD:H16	2:A:701:HGD:H11	1.63	0.42
1:A:67:MSE:HE3	1:B:298:VAL:CG2	2.47	0.42
1:A:123:ARG:HG3	1:A:339:ILE:HA	2.01	0.42
1:A:305:ASN:O	1:A:309:THR:HG23	2.20	0.42
1:A:163:ALA:HB3	1:A:164:PRO:HD3	2.01	0.42
1:A:186:THR:O	1:A:190:LEU:HG	2.19	0.42
1:A:206:ARG:HG2	1:A:264:SER:OG	2.20	0.42
1:B:171:ALA:O	1:B:175:ILE:HG13	2.19	0.42
1:A:512:LEU:HD23	1:A:512:LEU:HA	1.93	0.41
3:A:703:LDA:HM11	3:A:703:LDA:H22	1.83	0.41
1:A:100:LEU:O	1:A:104:VAL:HG23	2.21	0.41
1:A:228:LEU:HD23	1:A:228:LEU:HA	1.94	0.41
1:A:297:THR:HG23	1:A:300:ASP:N	2.34	0.41
1:A:561:ASP:OD1	1:A:561:ASP:N	2.41	0.41
1:B:449:ASP:OD1	1:B:450:THR:N	2.45	0.41
1:A:30:ALA:HA	1:A:36:ARG:NH1	2.35	0.41
1:A:202:ILE:HG21	1:A:268:LEU:HB2	2.03	0.41
1:A:374:ARG:NH1	1:A:376:ILE:HD11	2.35	0.41
1:B:81:LEU:HD23	1:B:81:LEU:HA	1.88	0.41
1:A:288:VAL:HG21	1:B:80:ALA:HB1	2.01	0.41
1:B:69:LEU:N	1:B:70:GLY:HA3	2.36	0.41
1:B:181:GLY:HA3	1:B:182:LEU:HA	1.83	0.41
1:B:372:ARG:HA	1:B:414:TRP:CH2	2.56	0.41
1:B:459:ARG:NH2	1:B:466:GLU:OE2	2.43	0.40
1:A:154:MSE:CB	1:A:325:ILE:HA	2.51	0.40
1:A:120:VAL:O	1:A:124:LEU:HG	2.22	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LEU:HD23	1:A:100:LEU:HA	1.94	0.40
1:B:137:THR:O	1:B:141:THR:OG1	2.34	0.40
1:B:311:LEU:HD23	1:B:312:PHE:CE1	2.56	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:ARG:NH2	1:B:591:GLU:OE1[4_547]	2.08	0.12
5:A:855:HOH:O	5:B:824:HOH:O[4_547]	2.11	0.09

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	598/614 (97%)	591 (99%)	7 (1%)	0	100	100
1	B	596/614 (97%)	581 (98%)	15 (2%)	0	100	100
All	All	1194/1228 (97%)	1172 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	478/478 (100%)	472 (99%)	6 (1%)	69	87
1	B	477/478 (100%)	470 (98%)	7 (2%)	65	85
All	All	955/956 (100%)	942 (99%)	13 (1%)	67	86

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	60	TYR
1	A	69	LEU
1	A	84	VAL
1	A	154	MSE
1	A	307	TYR
1	A	556	LEU
1	B	60	TYR
1	B	101	ARG
1	B	123	ARG
1	B	154	MSE
1	B	190	LEU
1	B	307	TYR
1	B	332	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	74	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

9 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	$\#\|Z\| > 2$
3	LDA	B	702	-	13,15,15	2.30	2 (15%)	14,17,17	0.45	0
3	LDA	A	702	-	13,15,15	2.28	2 (15%)	14,17,17	0.70	0
4	PO4	A	704	-	4,4,4	0.94	0	6,6,6	0.51	0
3	LDA	A	703	-	13,15,15	2.26	2 (15%)	14,17,17	0.67	0
4	PO4	B	704	-	4,4,4	0.96	0	6,6,6	0.44	0
3	LDA	B	701	-	13,15,15	2.45	2 (15%)	14,17,17	0.48	0
4	PO4	B	703	-	4,4,4	0.90	0	6,6,6	0.56	0
4	PO4	A	705	-	4,4,4	0.97	0	6,6,6	0.51	0
2	HGD	A	701	-	36,40,40	1.99	5 (13%)	40,51,51	1.32	6 (15%)

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	LDA	B	702	-	-	8/13/13/13	-
3	LDA	A	702	-	-	4/13/13/13	-
3	LDA	A	703	-	-	7/13/13/13	-
3	LDA	B	701	-	-	8/13/13/13	-
2	HGD	A	701	-	-	12/48/52/52	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	703	LDA	O1-N1	-6.93	1.25	1.42
3	B	701	LDA	O1-N1	-6.89	1.25	1.42
3	B	702	LDA	O1-N1	-6.65	1.25	1.42
3	A	702	LDA	O1-N1	-6.65	1.25	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	HGD	CD1-N2	5.56	1.45	1.34
3	B	701	LDA	C1-N1	-5.48	1.45	1.51
2	A	701	HGD	C5-N4	5.41	1.46	1.33
2	A	701	HGD	CD6-N5	4.90	1.44	1.34
2	A	701	HGD	C2-N3	4.90	1.45	1.33
3	B	702	LDA	C1-N1	-4.83	1.46	1.51
3	A	702	LDA	C1-N1	-4.70	1.46	1.51
3	A	703	LDA	C1-N1	-4.16	1.47	1.51
2	A	701	HGD	CG1-CD1	2.11	1.55	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	HGD	CG1-CD1-N2	2.76	120.72	115.86
2	A	701	HGD	CG6-CD6-N5	2.67	120.56	115.86
2	A	701	HGD	CB5-CA5-C5	2.26	114.56	109.46
2	A	701	HGD	O6-CD6-CG6	-2.17	118.09	122.02
2	A	701	HGD	O1-CD1-CG1	-2.11	118.19	122.02
2	A	701	HGD	CB6-CG6-CD6	-2.02	108.56	113.06

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	HGD	OE3-C3-CA3-N3
2	A	701	HGD	N6-CA6-CB6-CG6
3	A	703	LDA	C2-C1-N1-O1
3	A	703	LDA	C2-C1-N1-CM1
3	A	703	LDA	C2-C1-N1-CM2
3	B	702	LDA	C2-C1-N1-CM2
2	A	701	HGD	O2-C2-N3-CA3
2	A	701	HGD	CA2-C2-N3-CA3
2	A	701	HGD	CA6-CB6-CG6-CD6
2	A	701	HGD	OE4-C3-CA3-N3
3	B	701	LDA	C3-C4-C5-C6
3	B	702	LDA	C11-C10-C9-C8
3	B	702	LDA	C1-C2-C3-C4
3	B	701	LDA	C11-C10-C9-C8
3	A	703	LDA	C9-C10-C11-C12
3	A	702	LDA	C5-C6-C7-C8
3	A	703	LDA	C3-C4-C5-C6
3	B	701	LDA	C4-C5-C6-C7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	702	LDA	C7-C8-C9-C10
3	B	701	LDA	C7-C8-C9-C10
3	B	701	LDA	C5-C6-C7-C8
3	A	703	LDA	C11-C10-C9-C8
3	B	702	LDA	C3-C4-C5-C6
2	A	701	HGD	C6-CA6-CB6-CG6
3	B	702	LDA	C5-C6-C7-C8
3	B	702	LDA	C2-C1-N1-CM1
3	B	701	LDA	C1-C2-C3-C4
3	B	702	LDA	C2-C1-N1-O1
3	A	702	LDA	C9-C10-C11-C12
2	A	701	HGD	OE8-C6-CA6-CB6
2	A	701	HGD	CA1-CB1-CG1-CD1
3	A	702	LDA	C1-C2-C3-C4
3	B	701	LDA	C9-C10-C11-C12
2	A	701	HGD	O2-C2-CA2-N2
3	B	702	LDA	C7-C8-C9-C10
2	A	701	HGD	OE7-C6-CA6-CB6
2	A	701	HGD	N3-C2-CA2-N2
3	A	703	LDA	C1-C2-C3-C4
3	B	701	LDA	C2-C3-C4-C5

There are no ring outliers.

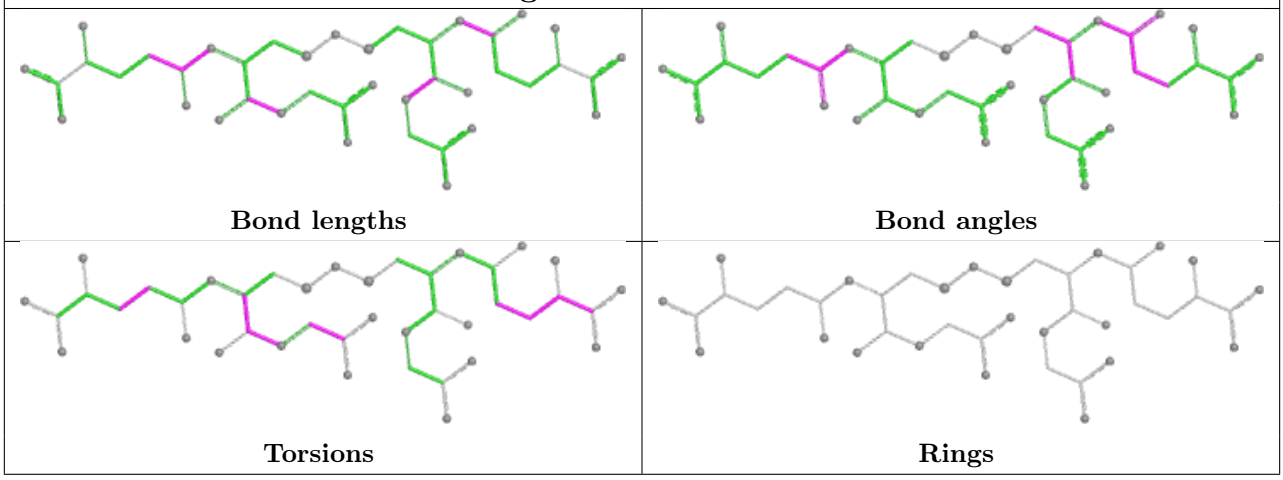
7 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	LDA	5	0
3	A	702	LDA	7	0
3	A	703	LDA	1	0
4	B	704	PO4	1	0
3	B	701	LDA	1	0
4	A	705	PO4	1	0
2	A	701	HGD	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 HGD A 701



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	588/614 (95%)	0.15	25 (4%)	35	38	30, 58, 95, 133	0
1	B	586/614 (95%)	0.22	23 (3%)	39	42	26, 55, 97, 164	0
All	All	1174/1228 (95%)	0.19	48 (4%)	37	40	26, 57, 96, 164	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	72	GLY	21.0
1	B	71	GLY	12.5
1	B	73	ALA	9.3
1	B	70	GLY	6.4
1	B	74	GLN	5.9
1	A	604	SER	5.2
1	A	494	ARG	4.7
1	A	136	ARG	4.4
1	A	603	VAL	4.2
1	A	137	THR	4.1
1	B	11	ASP	4.1
1	A	605	GLU	4.0
1	A	138	GLY	3.9
1	A	133	LEU	3.7
1	A	601	ALA	3.7
1	B	13	ARG	3.6
1	B	138	GLY	3.6
1	A	132	HIS	3.5
1	B	133	LEU	3.4
1	B	604	SER	3.3
1	A	177	TRP	3.3
1	B	136	ARG	3.2
1	B	14	HIS	3.2
1	B	137	THR	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	32	ASN	3.1
1	A	9	PRO	3.0
1	A	14	HIS	2.9
1	A	602	GLU	2.7
1	B	76	ALA	2.6
1	B	75	PRO	2.6
1	B	601	ALA	2.6
1	A	134	ALA	2.5
1	A	17	TRP	2.4
1	A	267	LEU	2.4
1	A	607	ALA	2.3
1	B	21	LYS	2.3
1	B	605	GLU	2.3
1	B	12	ALA	2.3
1	A	205	TRP	2.3
1	B	181	GLY	2.2
1	A	482	ARG	2.2
1	A	580	LEU	2.2
1	B	480	ILE	2.1
1	A	464	ARG	2.1
1	B	209	LEU	2.1
1	A	472	LYS	2.1
1	B	484	PRO	2.0
1	A	135	ARG	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 monosaccharides in this entry.

6.4 Ligands (i)

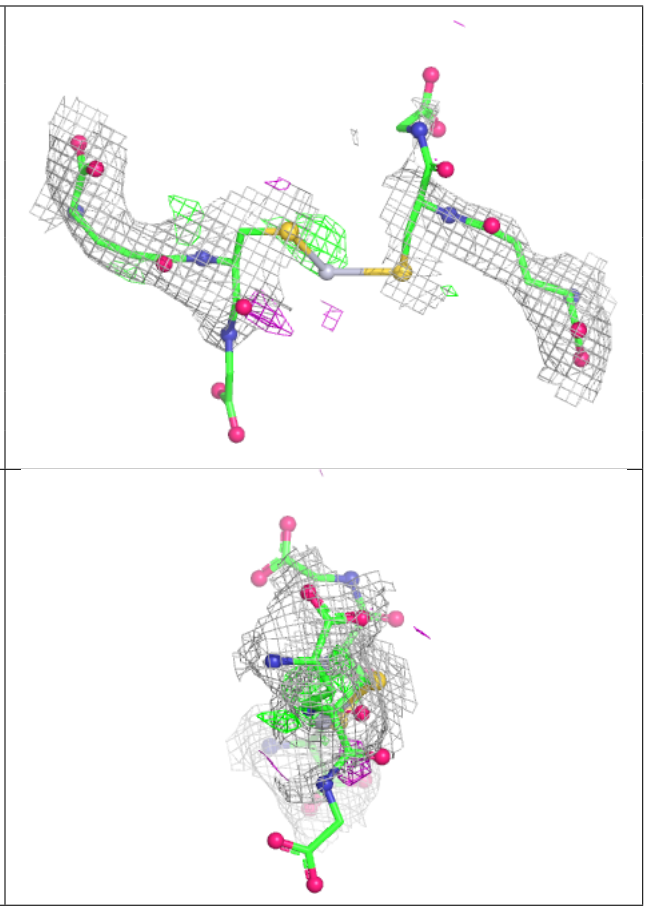
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PO4	A	705	5/5	0.69	0.41	148,148,149,149	0
3	LDA	A	702	16/16	0.75	0.40	60,69,83,84	0
3	LDA	B	702	16/16	0.79	0.27	59,64,81,82	0
2	HGD	A	701	41/41	0.79	0.48	34,103,115,274	41
4	PO4	B	704	5/5	0.80	0.31	157,157,157,158	0
4	PO4	B	703	5/5	0.85	0.17	112,116,117,118	0
4	PO4	A	704	5/5	0.88	0.13	113,115,115,115	0
3	LDA	A	703	16/16	0.92	0.32	56,58,65,65	0
3	LDA	B	701	16/16	0.96	0.37	44,52,61,62	16

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 HGD A 701:

$2mF_o$-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.