



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 11:53 am BST

PDB ID : 4EQ4  
Title : Crystal structure of seleno-methionine derivatized GH3.12  
Authors : Zubieta, C.; Nanao, M.; Jez, J.; Westfall, C.; Kapp, U.  
Deposited on : 2012-04-18  
Resolution : 2.07 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (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

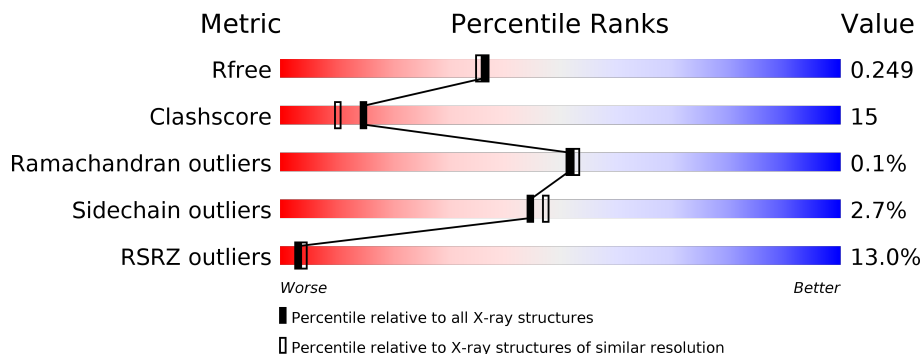
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.07 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	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	581	
1	B	581	

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 9183 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.

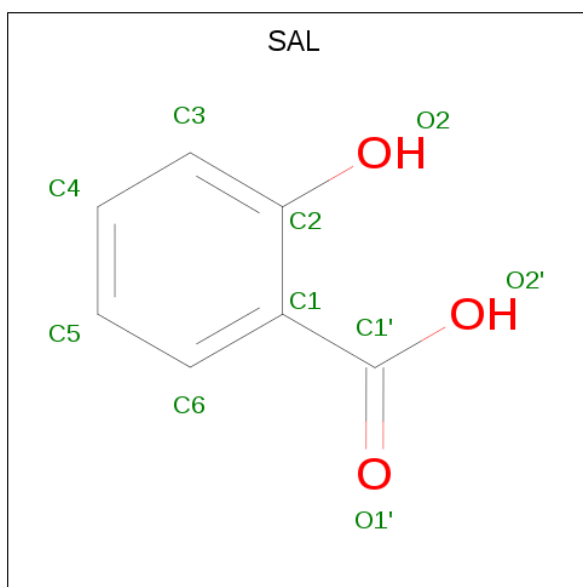
- Molecule 1 is a protein called 4-substituted benzoates-glutamate ligase GH3.12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	545	4277	2717	701	831	13	15	0	6	0
1	B	531	4177	2656	683	810	14	14	0	6	0

There are 12 discrepancies between the modelled and reference sequences:

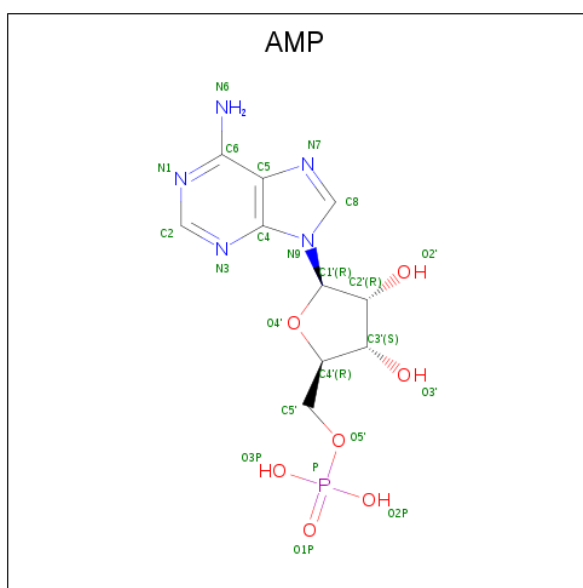
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	EXPRESSION TAG	UNP Q9LYU4
A	-4	SER	-	EXPRESSION TAG	UNP Q9LYU4
A	-3	HIS	-	EXPRESSION TAG	UNP Q9LYU4
A	-2	MSE	-	EXPRESSION TAG	UNP Q9LYU4
A	-1	ALA	-	EXPRESSION TAG	UNP Q9LYU4
A	0	SER	-	EXPRESSION TAG	UNP Q9LYU4
B	-5	GLY	-	EXPRESSION TAG	UNP Q9LYU4
B	-4	SER	-	EXPRESSION TAG	UNP Q9LYU4
B	-3	HIS	-	EXPRESSION TAG	UNP Q9LYU4
B	-2	MSE	-	EXPRESSION TAG	UNP Q9LYU4
B	-1	ALA	-	EXPRESSION TAG	UNP Q9LYU4
B	0	SER	-	EXPRESSION TAG	UNP Q9LYU4

- Molecule 2 is 2-HYDROXYBENZOIC ACID (three-letter code: SAL) (formula: C<sub>7</sub>H<sub>6</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	7	3		
2	B	1	Total	C	O	0	0
			10	7	3		

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula:  $C_{10}H_{14}N_5O_7P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

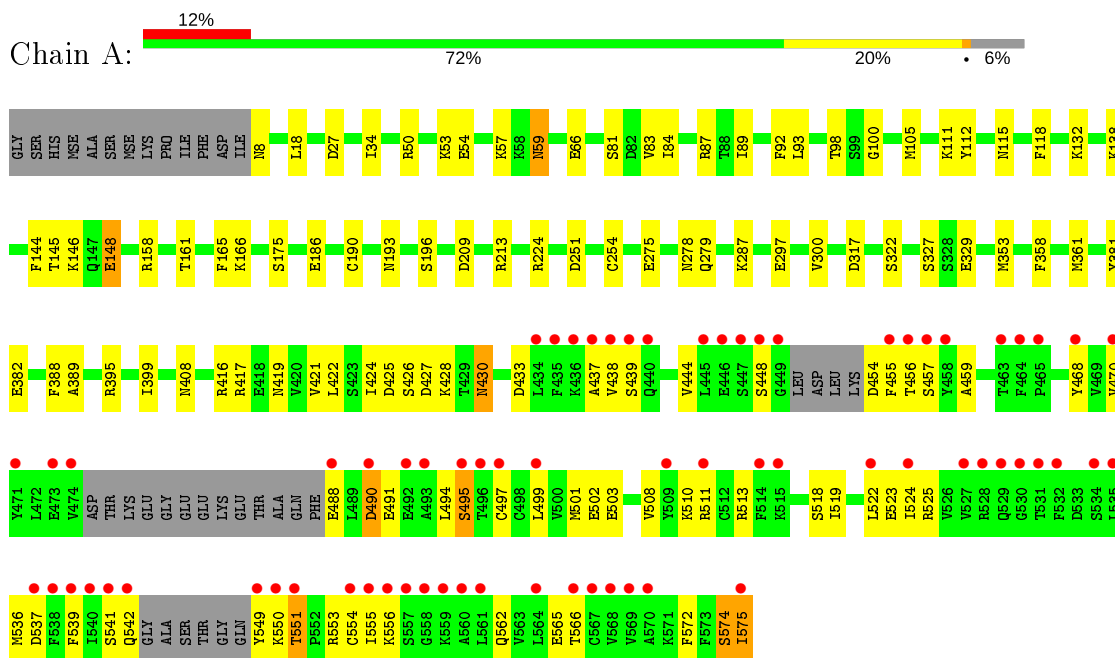
- Molecule 4 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	A	351	Total 351	O 351	0	0
4	B	312	Total 312	O 312	0	0

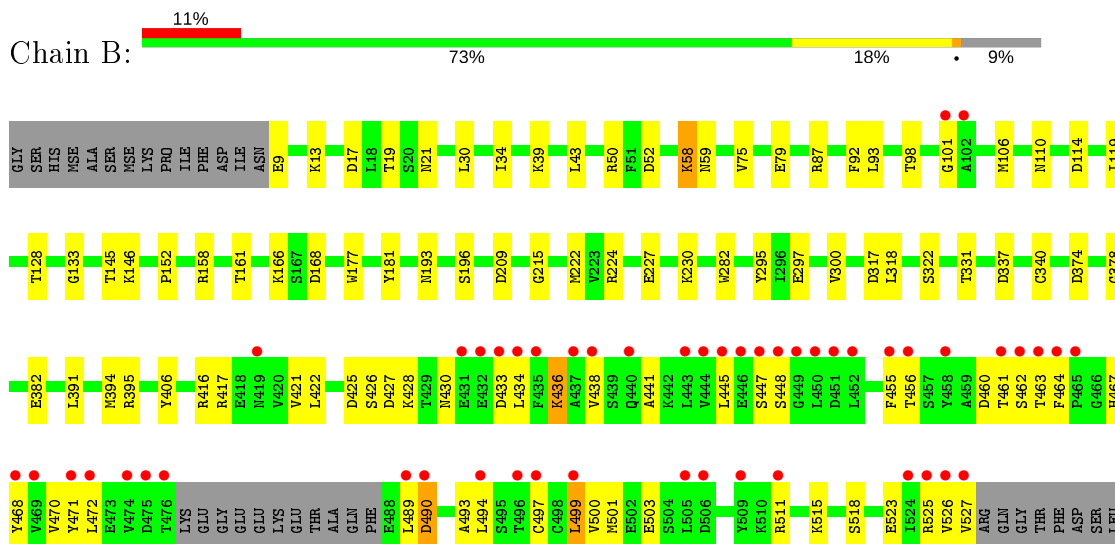
### 3 Residue-property plots

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: 4-substituted benzoates-glutamate ligase GH3.12



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MSE	ASP	PHE	ILE	SER	GLN	GLY	ALA	SER	THR	GLY	GLN	TYR	LYS	T551	P552	R553	C554	I555	R556	S557	G558	K559	A560	L561	Q562	V563	L564	E565	T566	C567	V568	V569	A570	F573	SER	ILE
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.86Å 66.30Å 100.45Å 90.00° 106.63° 90.00°	Depositor
Resolution (Å)	56.97 – 2.07 56.96 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.1 (56.97-2.07) 99.1 (56.96-2.08)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.25	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 2.08Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, $R_{free}$	0.214 , 0.252 0.210 , 0.249	Depositor DCC
$R_{free}$ test set	3486 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.7	Xtrriage
Anisotropy	0.136	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 48.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9183	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.66	1/4366 (0.0%)	0.69	0/5896
1	B	0.66	0/4266	0.69	1/5767 (0.0%)
All	All	0.66	1/8632 (0.0%)	0.69	1/11663 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	SER	CB-OG	-5.37	1.35	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	110	ASN	CB-CA-C	-5.65	99.09	110.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4277	0	4119	159	1
1	B	4177	0	4062	113	1
2	A	10	0	5	0	0
2	B	10	0	5	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	23	0	12	0	0
3	B	23	0	12	0	0
4	A	351	0	0	34	0
4	B	312	0	0	27	0
All	All	9183	0	8215	255	1

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 15.

All (255) 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:438:VAL:CG2	1:A:501:MSE:HE1	1.27	1.56
1:B:455:PHE:CB	1:B:553:ARG:HH12	1.23	1.46
1:A:438:VAL:CG2	1:A:501:MSE:CE	1.97	1.41
1:A:438:VAL:HG22	1:A:501:MSE:CE	1.64	1.23
1:A:146:LYS:HE2	1:A:511:ARG:NH2	1.52	1.22
1:A:438:VAL:HG23	1:A:501:MSE:CE	1.61	1.22
1:B:455:PHE:CB	1:B:553:ARG:NH1	2.06	1.17
1:A:502:GLU:HG3	1:A:522:LEU:HD12	1.22	1.14
1:A:510:LYS:HZ1	1:B:499:LEU:HD13	1.02	1.11
1:A:502:GLU:CG	1:A:522:LEU:HD12	1.82	1.09
1:A:510:LYS:NZ	1:B:499:LEU:HD13	1.69	1.08
1:B:438:VAL:HG21	1:B:553:ARG:HH22	1.19	1.07
1:A:438:VAL:HG23	1:A:501:MSE:HE1	1.07	1.06
1:A:499:LEU:HD21	1:A:575:ILE:H	1.19	1.06
1:B:317:ASP:C	4:B:952:HOH:O	1.95	1.05
1:B:438:VAL:HG21	1:B:553:ARG:NH2	1.70	1.05
1:A:416:ARG:CZ	4:A:1018:HOH:O	2.04	1.04
1:A:468:TYR:HB2	1:A:522:LEU:HD23	1.34	1.04
1:B:87:ARG:NH2	4:B:773:HOH:O	1.92	1.02
1:A:575:ILE:HD12	1:B:515:LYS:HD2	1.38	1.02
1:A:438:VAL:HG22	1:A:501:MSE:HE1	1.15	1.01
1:B:9:GLU:N	4:B:822:HOH:O	1.92	1.01
1:A:499:LEU:HD21	1:A:575:ILE:N	1.74	1.01
1:A:98:THR:O	4:A:1035:HOH:O	1.81	0.98
1:A:416:ARG:NE	4:A:1018:HOH:O	1.93	0.97
1:A:536:MSE:HG3	1:A:549:TYR:CD2	1.99	0.96
1:A:468:TYR:HB2	1:A:522:LEU:CD2	1.97	0.95
1:A:146:LYS:HE2	1:A:511:ARG:HH22	1.29	0.91
1:B:317:ASP:O	4:B:952:HOH:O	1.83	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:ASP:OD2	4:B:992:HOH:O	1.88	0.91
1:B:318:LEU:N	4:B:952:HOH:O	2.00	0.91
1:A:146:LYS:HE2	1:A:511:ARG:HH21	1.37	0.90
1:A:408:ASN:OD1	4:A:794:HOH:O	1.90	0.90
1:B:79:GLU:OE1	4:B:993:HOH:O	1.91	0.89
1:A:438:VAL:CG2	1:A:501:MSE:HE3	1.99	0.89
1:B:58:LYS:HG2	1:B:59:ASN:OD1	1.72	0.88
1:A:499:LEU:CD2	1:A:575:ILE:H	1.85	0.88
1:A:468:TYR:CB	1:A:522:LEU:HD23	2.05	0.87
1:A:317:ASP:O	4:A:1019:HOH:O	1.92	0.86
1:B:318:LEU:CA	4:B:952:HOH:O	2.24	0.86
1:A:575:ILE:HD12	1:B:515:LYS:CD	2.05	0.85
1:B:455:PHE:C	1:B:553:ARG:NH1	2.30	0.85
1:A:287:LYS:HE2	4:A:1037:HOH:O	1.77	0.84
1:B:318:LEU:HA	4:B:952:HOH:O	1.77	0.83
1:B:455:PHE:CA	1:B:553:ARG:NH1	2.40	0.83
1:A:510:LYS:NZ	1:B:499:LEU:HD22	1.92	0.83
1:A:146:LYS:NZ	4:A:947:HOH:O	2.13	0.82
1:B:374:ASP:OD2	4:B:983:HOH:O	1.97	0.82
1:A:499:LEU:HD23	1:A:574:SER:OG	1.80	0.81
1:A:27:ASP:OD1	1:A:53:LYS:NZ	2.12	0.81
1:B:455:PHE:CA	1:B:553:ARG:HH12	1.92	0.81
1:A:100:GLY:O	4:A:993:HOH:O	1.98	0.81
1:B:489:LEU:O	1:B:490:ASP:CB	2.30	0.80
1:B:114:ASP:HB2	4:B:986:HOH:O	1.83	0.79
1:A:455:PHE:HE1	1:A:553:ARG:HD2	1.48	0.79
1:A:209:ASP:OD1	4:A:987:HOH:O	2.00	0.78
1:A:438:VAL:CA	1:A:501:MSE:HE3	2.13	0.78
1:A:327:SER:O	4:A:1027:HOH:O	2.00	0.78
1:A:66[B]:GLU:OE2	4:A:976:HOH:O	1.98	0.77
1:A:287:LYS:NZ	4:A:922:HOH:O	2.18	0.76
1:A:510:LYS:NZ	1:B:499:LEU:CD1	2.48	0.75
1:A:499:LEU:HD21	1:A:575:ILE:CA	2.16	0.75
1:A:510:LYS:HZ3	1:B:499:LEU:HD22	1.50	0.74
1:A:287:LYS:CE	4:A:1037:HOH:O	2.34	0.74
1:A:499:LEU:HD11	1:A:575:ILE:O	1.87	0.74
1:A:275:GLU:OE2	1:A:279:GLN:NE2	2.21	0.74
1:A:213:ARG:NH1	1:A:297:GLU:OE1	2.21	0.73
1:B:224[B]:ARG:NH1	4:B:929:HOH:O	2.22	0.73
1:B:470:VAL:HG12	1:B:472:LEU:HD13	1.72	0.72
1:A:419:ASN:OD1	4:A:815:HOH:O	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:VAL:HG23	1:B:422:LEU:HG	1.71	0.71
1:A:565:GLU:HA	4:A:1028:HOH:O	1.89	0.71
1:A:455:PHE:CE1	1:A:553:ARG:HD2	2.25	0.71
1:A:536:MSE:HG3	1:A:549:TYR:CE2	2.26	0.71
1:B:455:PHE:C	1:B:553:ARG:HH11	1.93	0.71
1:A:499:LEU:HD11	1:A:575:ILE:C	2.11	0.70
1:A:424:ILE:HD11	1:A:459:ALA:HB1	1.73	0.70
1:A:317:ASP:C	4:A:1019:HOH:O	2.28	0.70
1:A:468:TYR:CB	1:A:522:LEU:CD2	2.66	0.70
1:A:457:SER:OG	1:A:553:ARG:O	2.10	0.70
1:A:502:GLU:HG3	1:A:522:LEU:CD1	2.12	0.69
1:A:416:ARG:NH2	4:A:1018:HOH:O	2.20	0.69
1:A:382:GLU:OE1	1:A:395:ARG:NH2	2.26	0.68
1:A:287:LYS:NZ	4:A:1037:HOH:O	2.26	0.67
1:A:438:VAL:HA	1:A:501:MSE:HE3	1.74	0.67
1:B:300:VAL:HG22	1:B:322:SER:HB2	1.77	0.67
1:B:19:THR:OG1	4:B:897:HOH:O	1.85	0.66
1:B:427:ASP:OD2	1:B:468:TYR:OH	2.09	0.66
1:A:497:CYS:O	1:A:501:MSE:HG3	1.94	0.66
1:A:551:THR:HG22	1:A:553:ARG:NH1	2.11	0.65
1:B:526:VAL:O	1:B:568:VAL:HA	1.96	0.65
1:B:50:ARG:NE	4:B:873:HOH:O	2.24	0.65
1:B:422:LEU:HD13	1:B:468:TYR:CD2	2.32	0.64
1:A:427:ASP:OD1	1:A:519:ILE:HD11	1.97	0.64
1:B:455:PHE:O	1:B:553:ARG:NH1	2.29	0.63
1:A:438:VAL:N	1:A:501:MSE:HE3	2.14	0.63
1:B:421:VAL:HB	1:B:554:CYS:HB2	1.80	0.63
1:A:437:ALA:HB1	1:A:501:MSE:HA	1.80	0.63
1:A:510:LYS:HZ1	1:B:499:LEU:CD1	1.94	0.62
1:B:434:LEU:O	1:B:434:LEU:HD12	1.99	0.62
1:A:470:VAL:CG1	1:A:524:ILE:HG12	2.28	0.62
1:B:224[B]:ARG:HG3	1:B:464:PHE:HZ	1.63	0.62
1:A:148:GLU:OE1	1:A:158:ARG:NH2	2.31	0.62
1:A:551:THR:HG22	1:A:553:ARG:HH11	1.64	0.62
1:A:87:ARG:NH2	4:A:819:HOH:O	2.31	0.60
1:B:489:LEU:CB	1:B:494:LEU:HD11	2.31	0.60
1:B:119:ILE:HG13	1:B:331:THR:HG21	1.83	0.60
1:A:424:ILE:O	1:A:427:ASP:OD1	2.18	0.60
1:A:161[B]:THR:HB	4:A:924:HOH:O	2.02	0.59
1:A:422:LEU:HD21	1:A:457:SER:HB2	1.85	0.59
1:A:490:ASP:N	1:A:490:ASP:OD2	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:568:VAL:O	1:B:568:VAL:HG22	2.03	0.59
1:A:502:GLU:HG2	1:A:522:LEU:HD12	1.80	0.58
1:A:146:LYS:CE	1:A:511:ARG:HH21	2.13	0.58
1:A:456:THR:OG1	1:A:457:SER:N	2.37	0.58
1:A:224[A]:ARG:HD2	4:A:986:HOH:O	2.03	0.58
1:A:510:LYS:NZ	1:B:499:LEU:CD2	2.64	0.57
1:A:83:VAL:HG12	1:A:84:ILE:HG23	1.86	0.57
1:B:168:ASP:OD1	4:B:996:HOH:O	2.17	0.57
1:A:224[B]:ARG:HD2	4:A:986:HOH:O	2.04	0.57
1:B:470:VAL:HG12	1:B:472:LEU:CD1	2.34	0.57
1:A:494:LEU:HD22	1:A:572:PHE:CE2	2.40	0.57
1:B:161[B]:THR:HG23	4:B:714:HOH:O	2.03	0.57
1:A:562:GLN:O	1:A:566:THR:HG23	2.05	0.57
1:A:161[B]:THR:HG22	4:A:720:HOH:O	2.02	0.57
1:A:190:CYS:HB3	1:A:196:SER:HB3	1.86	0.57
1:A:224[B]:ARG:NH1	4:A:995:HOH:O	2.37	0.57
1:A:224[A]:ARG:NH1	4:A:995:HOH:O	2.38	0.56
1:A:111:LYS:HG2	1:A:388:PHE:CG	2.40	0.56
1:B:499:LEU:CD1	1:B:503:GLU:OE2	2.53	0.56
1:A:510:LYS:HZ2	1:B:499:LEU:HD22	1.69	0.56
1:A:144:PHE:HB3	1:A:193:ASN:ND2	2.21	0.56
1:B:445:LEU:O	1:B:448:SER:N	2.39	0.56
1:A:112:TYR:OH	4:A:1027:HOH:O	2.17	0.55
1:A:425:ASP:CG	1:A:426:SER:H	2.10	0.55
1:B:30:LEU:O	1:B:34:ILE:HG12	2.06	0.55
1:A:209:ASP:OD2	4:A:981:HOH:O	2.18	0.55
1:B:499:LEU:CD1	1:B:503:GLU:CD	2.75	0.55
1:A:213:ARG:NE	4:A:921:HOH:O	2.31	0.55
1:B:417:ARG:HD3	1:B:428:LYS:HD3	1.88	0.55
1:B:499:LEU:C	1:B:499:LEU:HD12	2.28	0.54
1:A:146:LYS:CE	1:A:511:ARG:NH2	2.47	0.54
1:A:18:LEU:HD11	1:A:118:PHE:HZ	1.72	0.54
1:A:575:ILE:CD1	1:B:515:LYS:CD	2.82	0.53
1:B:430:ASN:OD1	1:B:433:ASP:N	2.42	0.53
1:B:499:LEU:HG	1:B:500:VAL:N	2.24	0.53
1:B:406:TYR:HE2	4:B:897:HOH:O	1.91	0.53
1:B:224[B]:ARG:HH11	1:B:518:SER:HB3	1.73	0.53
1:A:424:ILE:CD1	1:A:459:ALA:HB1	2.39	0.52
1:A:455:PHE:CE1	1:A:553:ARG:CD	2.92	0.52
1:A:275:GLU:O	1:A:275:GLU:OE2	2.27	0.52
1:A:499:LEU:HD21	1:A:575:ILE:C	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:ILE:HD11	1:B:511:ARG:HA	1.92	0.52
1:A:502:GLU:CG	1:A:522:LEU:CD1	2.73	0.51
1:B:499:LEU:HD13	1:B:503:GLU:OE2	2.11	0.51
1:A:361:MSE:HG3	1:A:399:ILE:HD12	1.93	0.51
1:A:575:ILE:HD13	1:B:511:ARG:NE	2.25	0.51
1:B:224[B]:ARG:CZ	4:B:929:HOH:O	2.58	0.50
1:A:327:SER:OG	1:A:329:GLU:OE1	2.21	0.50
1:A:438:VAL:HG22	1:A:501:MSE:HE3	1.73	0.50
1:B:230:LYS:HE3	1:B:282:TRP:CD1	2.47	0.50
1:A:421:VAL:HB	1:A:554:CYS:HB3	1.93	0.50
1:B:227:GLU:HG3	1:B:464:PHE:CD1	2.46	0.49
1:A:554:CYS:O	1:A:555:ILE:HD13	2.13	0.49
1:B:378:GLY:HA2	4:B:798:HOH:O	2.13	0.49
1:B:224[B]:ARG:HG3	1:B:464:PHE:CZ	2.44	0.49
1:B:470:VAL:HG11	1:B:501:MSE:HE1	1.93	0.49
1:B:525:ARG:NH2	4:B:959:HOH:O	2.46	0.48
1:A:89:ILE:HD11	1:A:389:ALA:O	2.13	0.48
1:A:145:THR:HG21	1:A:166:LYS:HD3	1.95	0.48
1:B:133:GLY:HA2	4:B:990:HOH:O	2.12	0.48
1:B:441:ALA:O	1:B:445:LEU:HB2	2.13	0.48
1:A:502:GLU:OE2	1:A:513:ARG:NE	2.28	0.48
1:A:438:VAL:HG22	1:A:501:MSE:SE	2.61	0.48
1:B:295:TYR:CE1	1:B:297:GLU:HB2	2.48	0.48
1:A:382:GLU:OE2	1:A:395:ARG:HB3	2.13	0.47
1:A:536:MSE:HA	1:A:549:TYR:CZ	2.49	0.47
1:B:391:LEU:HD13	1:B:394:MSE:HE2	1.96	0.47
1:B:467:HIS:HE1	1:B:523:GLU:OE1	1.97	0.47
1:A:132:LYS:HB3	4:A:975:HOH:O	2.13	0.47
1:B:21:ASN:ND2	4:B:808:HOH:O	2.39	0.47
1:B:58:LYS:CG	1:B:59:ASN:OD1	2.54	0.47
1:A:503:GLU:HB3	1:B:503:GLU:CD	2.35	0.47
1:A:146:LYS:HE3	1:A:193:ASN:ND2	2.30	0.47
1:B:145:THR:HG21	1:B:166:LYS:HD3	1.96	0.47
1:B:445:LEU:HD13	1:B:497:CYS:SG	2.54	0.47
1:A:430:ASN:ND2	1:A:433:ASP:OD2	2.48	0.47
1:A:510:LYS:NZ	1:B:499:LEU:CG	2.78	0.47
1:A:358:PHE:HB3	1:A:381:TYR:HB3	1.98	0.46
1:B:215:GLY:HA2	1:B:222:MSE:SE	2.65	0.46
1:B:497:CYS:O	1:B:501:MSE:HG3	2.15	0.46
1:B:106:MSE:SE	1:B:394:MSE:HE1	2.64	0.46
1:A:508:VAL:O	1:A:511:ARG:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:TYR:CB	1:A:522:LEU:HD21	2.45	0.45
1:A:537:ASP:O	1:A:541:SER:N	2.32	0.45
1:A:575:ILE:HG23	1:B:511:ARG:HH21	1.81	0.45
1:B:75:VAL:HG12	1:B:92:PHE:HZ	1.81	0.45
1:A:300:VAL:HG22	1:A:322:SER:HB2	1.99	0.45
1:B:471:TYR:HA	1:B:525:ARG:O	2.17	0.45
1:A:132:LYS:HA	1:A:132:LYS:HD3	1.81	0.45
1:A:523:GLU:CD	1:A:525:ARG:HE	2.19	0.44
1:B:436:LYS:HD3	1:B:436:LYS:HA	1.72	0.44
1:B:526:VAL:O	1:B:568:VAL:CA	2.64	0.44
1:A:34:ILE:HA	1:A:34:ILE:HD13	1.82	0.44
1:A:417:ARG:HD3	1:A:428:LYS:HD3	1.99	0.44
1:B:13:LYS:HD3	1:B:17:ASP:OD1	2.17	0.44
1:A:490:ASP:HB3	1:B:152:PRO:HD3	1.99	0.44
1:B:490:ASP:O	1:B:494:LEU:HD12	2.18	0.44
1:B:499:LEU:HD12	1:B:503:GLU:CD	2.38	0.43
1:A:575:ILE:HD13	1:B:511:ARG:HE	1.83	0.43
1:A:161[B]:THR:HG23	1:A:165:PHE:CE2	2.52	0.43
1:A:470:VAL:HG13	1:A:524:ILE:HG12	1.98	0.43
1:A:93:LEU:HA	1:A:158:ARG:O	2.18	0.43
1:B:128[B]:THR:HG23	1:B:177:TRP:CZ2	2.54	0.43
1:B:374:ASP:OD2	4:B:797:HOH:O	2.21	0.43
1:A:138:LYS:HE2	4:A:916:HOH:O	2.19	0.43
1:B:417:ARG:NH2	4:B:735:HOH:O	2.50	0.43
1:A:186:GLU:N	1:A:186:GLU:OE1	2.45	0.43
1:B:527:VAL:HA	1:B:568:VAL:HA	1.99	0.43
1:A:454:ASP:OD1	1:A:455:PHE:N	2.49	0.43
1:A:539:PHE:HA	1:A:542:GLN:HB2	2.01	0.43
1:A:53:LYS:HE3	1:A:57:LYS:HE2	2.00	0.43
1:A:536:MSE:HA	1:A:549:TYR:CE2	2.53	0.43
1:A:92:PHE:HB3	1:A:105:MSE:HG2	2.01	0.43
1:A:502:GLU:HG3	1:A:522:LEU:HB2	2.00	0.43
1:A:444:VAL:O	1:A:448:SER:HB2	2.19	0.42
1:B:93:LEU:HA	1:B:158:ARG:O	2.20	0.42
1:A:132:LYS:HE3	4:A:909:HOH:O	2.20	0.42
1:A:251:ASP:OD2	1:A:254:CYS:N	2.44	0.42
1:A:499:LEU:HB3	1:A:503:GLU:OE2	2.20	0.42
1:B:460:ASP:CG	1:B:462:SER:HG	2.22	0.42
1:B:181:TYR:OH	4:B:879:HOH:O	2.15	0.42
1:B:472:LEU:HA	1:B:472:LEU:HD12	1.76	0.42
1:B:98:THR:OG1	1:B:101:GLY:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:MSE:HG3	1:A:399:ILE:CD1	2.50	0.42
1:A:115:ASN:HB3	1:A:353:MSE:SE	2.70	0.42
1:A:575:ILE:CD1	1:B:515:LYS:HD3	2.49	0.42
1:A:549:TYR:CG	1:A:550:LYS:N	2.87	0.41
1:B:382:GLU:OE2	1:B:395:ARG:HB3	2.21	0.41
1:A:491:GLU:O	1:A:495:SER:HB2	2.20	0.41
1:B:425:ASP:CG	1:B:426:SER:H	2.24	0.41
1:A:100:GLY:N	4:A:1015:HOH:O	2.52	0.41
1:B:43:LEU:HD23	1:B:43:LEU:HA	1.82	0.41
1:A:59:ASN:ND2	4:A:859:HOH:O	2.18	0.41
1:B:416:ARG:NE	4:B:909:HOH:O	2.46	0.41
1:A:224[B]:ARG:NH1	1:A:518:SER:HB3	2.36	0.41
1:B:193:ASN:HA	1:B:196:SER:OG	2.21	0.40
1:B:456:THR:O	1:B:471:TYR:N	2.54	0.40
1:A:224[B]:ARG:HD3	1:A:224[B]:ARG:HH11	1.77	0.40
1:A:491:GLU:O	1:A:491:GLU:HG2	2.22	0.40
1:B:493:ALA:HB3	1:B:494:LEU:HD12	2.02	0.40
1:A:224[A]:ARG:HH11	1:A:224[A]:ARG:HD3	1.77	0.40
1:B:337:ASP:OD2	1:B:340:CYS:HB3	2.21	0.40

All (1) 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:50:ARG:NH1	1:B:209:ASP:OD2[1_655]	1.78	0.42

## 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	543/581 (94%)	522 (96%)	21 (4%)	0	<b>100</b> <b>100</b>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	531/581 (91%)	515 (97%)	15 (3%)	1 (0%)	47	47
All	All	1074/1162 (92%)	1037 (97%)	36 (3%)	1 (0%)	51	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	490	ASP

### 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	472/510 (92%)	457 (97%)	15 (3%)	39	40
1	B	469/510 (92%)	459 (98%)	10 (2%)	53	57
All	All	941/1020 (92%)	916 (97%)	25 (3%)	44	47

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	54	GLU
1	A	59	ASN
1	A	148	GLU
1	A	175	SER
1	A	278	ASN
1	A	430	ASN
1	A	439	SER
1	A	488	GLU
1	A	490	ASP
1	A	495	SER
1	A	551	THR
1	A	556	LYS
1	A	574	SER
1	A	575	ILE

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Mol	Chain	Res	Type
1	B	39	LYS
1	B	58	LYS
1	B	146	LYS
1	B	436	LYS
1	B	447	SER
1	B	461	THR
1	B	463	THR
1	B	499	LEU
1	B	568	VAL
1	B	569	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	193	ASN
1	A	247	ASN
1	B	110	ASN
1	B	467	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](#)

4 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	SAL	A	601	-	8,10,10	1.12	1 (12%)	9,13,13	0.79	0
3	AMP	B	602	-	22,25,25	0.79	1 (4%)	25,38,38	1.27	5 (20%)
2	SAL	B	601	-	8,10,10	1.20	1 (12%)	9,13,13	0.79	0
3	AMP	A	602	-	22,25,25	0.80	1 (4%)	25,38,38	1.31	4 (16%)

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	SAL	A	601	-	-	0/0/4/4	0/1/1/1
3	AMP	B	602	-	-	3/6/26/26	0/3/3/3
2	SAL	B	601	-	-	0/0/4/4	0/1/1/1
3	AMP	A	602	-	-	1/6/26/26	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	SAL	C1-C1'	2.81	1.50	1.47
2	B	601	SAL	C1-C1'	2.75	1.50	1.47
3	B	602	AMP	C5-C4	2.28	1.47	1.40
3	A	602	AMP	C5-C4	2.21	1.46	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	AMP	N3-C2-N1	-3.23	123.63	128.68
3	A	602	AMP	N3-C2-N1	-3.14	123.76	128.68
3	A	602	AMP	N6-C6-N1	2.55	123.86	118.57
3	B	602	AMP	C1'-N9-C4	-2.53	122.19	126.64
3	A	602	AMP	C2-N1-C6	2.31	122.71	118.75
3	B	602	AMP	N6-C6-N1	2.20	123.14	118.57
3	B	602	AMP	C2-N1-C6	2.05	122.27	118.75
3	B	602	AMP	O2P-P-O1P	2.02	118.58	110.68
3	A	602	AMP	O2P-P-O1P	2.01	118.55	110.68

There are no chirality outliers.

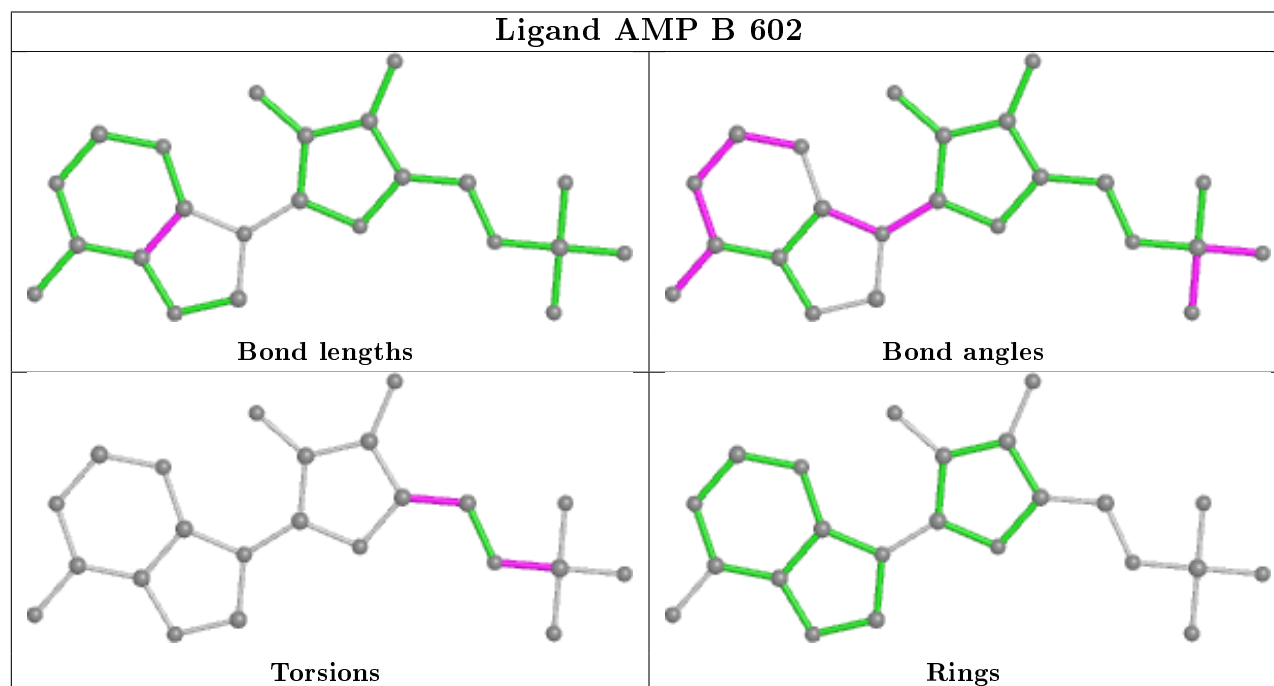
All (4) torsion outliers are listed below:

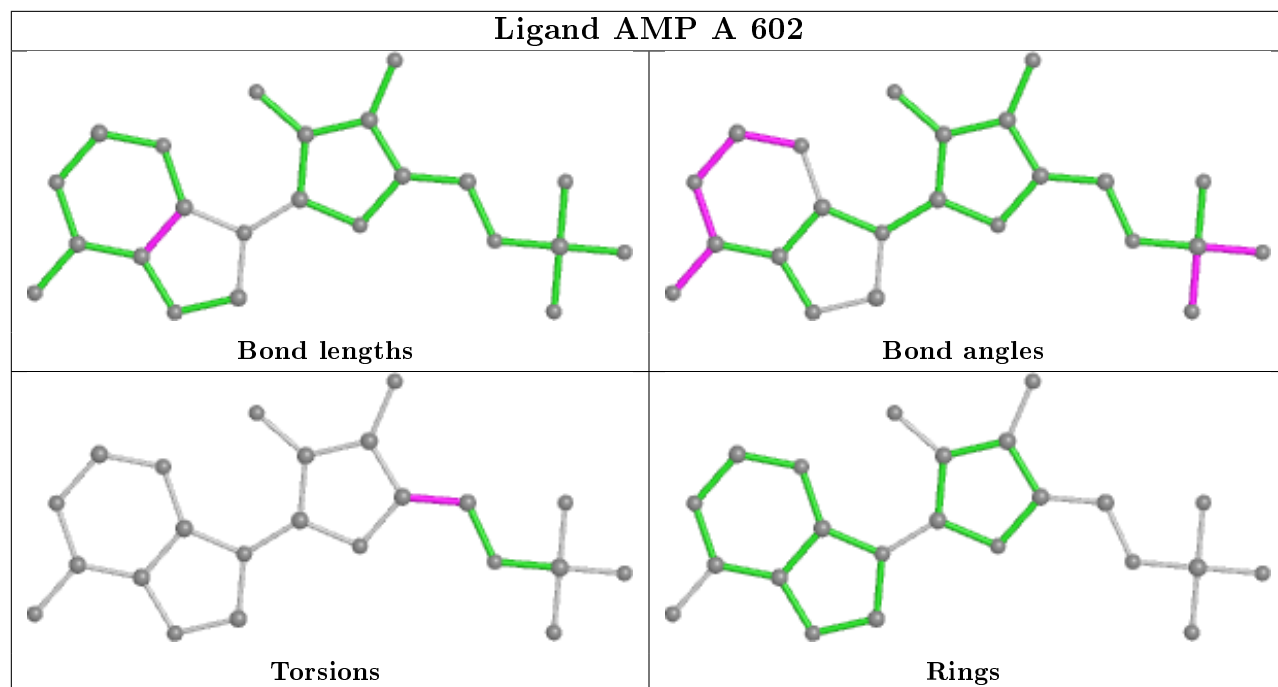
Mol	Chain	Res	Type	Atoms
3	B	602	AMP	O4'-C4'-C5'-O5'
3	B	602	AMP	C3'-C4'-C5'-O5'
3	B	602	AMP	C5'-O5'-P-O2P
3	A	602	AMP	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	530/581 (91%)	0.52	70 (13%) 3 4	10, 21, 88, 114	0
1	B	517/581 (88%)	0.60	66 (12%) 3 4	14, 26, 93, 112	0
All	All	1047/1162 (90%)	0.56	136 (12%) 3 4	10, 24, 91, 114	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	541	SER	10.6
1	B	475	ASP	9.4
1	B	559	LYS	9.4
1	A	532	PHE	9.0
1	B	489	LEU	9.0
1	B	452	LEU	8.7
1	B	560	ALA	8.5
1	B	449	GLY	8.3
1	B	434	LEU	8.0
1	B	476	THR	7.9
1	B	555	ILE	7.7
1	A	540	ILE	7.7
1	B	450	LEU	7.5
1	A	539	PHE	7.3
1	A	558	GLY	7.1
1	A	435	PHE	7.1
1	A	549	TYR	6.8
1	B	564	LEU	6.1
1	B	451	ASP	6.1
1	A	448	SER	6.0
1	A	527	VAL	5.8
1	A	455	PHE	5.8
1	B	569	VAL	5.8
1	A	564	LEU	5.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	568	VAL	5.7
1	A	551	THR	5.7
1	A	535	LEU	5.6
1	A	456	THR	5.5
1	B	463	THR	5.5
1	B	474	VAL	5.5
1	B	445	LEU	5.4
1	B	438	VAL	5.3
1	B	494	LEU	5.3
1	A	474	VAL	5.2
1	A	575	ILE	5.2
1	A	566	THR	5.1
1	A	568	VAL	5.1
1	A	463	THR	5.0
1	B	437	ALA	4.8
1	B	558	GLY	4.8
1	A	560	ALA	4.8
1	B	499	LEU	4.7
1	B	471	TYR	4.7
1	A	557	SER	4.7
1	A	538	PHE	4.6
1	B	566	THR	4.6
1	B	455	PHE	4.6
1	A	449	GLY	4.5
1	B	567	CYS	4.4
1	A	550	LYS	4.4
1	B	443	LEU	4.4
1	A	446	GLU	4.3
1	B	557	SER	4.3
1	A	497	CYS	4.2
1	A	567	CYS	4.2
1	B	465	PRO	4.1
1	B	561	LEU	4.1
1	B	458	TYR	4.1
1	B	526	VAL	4.1
1	A	530	GLY	4.0
1	A	522	LEU	4.0
1	A	438	VAL	4.0
1	B	444	VAL	3.9
1	B	435	PHE	3.9
1	A	492	GLU	3.7
1	A	439	SER	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	464	PHE	3.6
1	A	570	ALA	3.6
1	A	528	ARG	3.6
1	A	499	LEU	3.5
1	A	569	VAL	3.5
1	B	101	GLY	3.4
1	A	515	LYS	3.3
1	A	555	ILE	3.3
1	B	562	GLN	3.2
1	A	457	SER	3.2
1	B	570	ALA	3.1
1	B	447	SER	3.1
1	A	488	GLU	3.1
1	B	102	ALA	3.1
1	B	433	ASP	2.9
1	A	447	SER	2.9
1	B	553	ARG	2.9
1	A	531	THR	2.9
1	B	461	THR	2.8
1	A	465	PRO	2.8
1	B	440	GLN	2.8
1	B	490	ASP	2.8
1	A	496	THR	2.8
1	A	445	LEU	2.7
1	B	509	TYR	2.7
1	A	493	ALA	2.7
1	B	525	ARG	2.7
1	B	431	GLU	2.7
1	A	464	PHE	2.7
1	B	456	THR	2.6
1	A	554	CYS	2.6
1	B	432	GLU	2.6
1	B	524	ILE	2.6
1	A	514	PHE	2.6
1	A	542	GLN	2.6
1	A	470	VAL	2.5
1	A	471	TYR	2.5
1	A	509	TYR	2.5
1	A	436	LYS	2.5
1	B	552	PRO	2.4
1	A	537	ASP	2.4
1	B	446	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	561	LEU	2.4
1	A	529	GLN	2.4
1	B	469	VAL	2.4
1	A	440	GLN	2.3
1	B	448	SER	2.3
1	A	458	TYR	2.3
1	B	419	ASN	2.3
1	A	495	SER	2.3
1	A	524	ILE	2.3
1	A	434	LEU	2.3
1	A	511	ARG	2.3
1	B	496	THR	2.2
1	A	534	SER	2.2
1	A	490	ASP	2.2
1	B	551	THR	2.2
1	A	437	ALA	2.2
1	B	472	LEU	2.2
1	A	473	GLU	2.1
1	B	468	TYR	2.1
1	B	462	SER	2.1
1	A	468	TYR	2.1
1	B	497	CYS	2.1
1	B	506	ASP	2.1
1	A	559	LYS	2.1
1	B	511	ARG	2.0
1	B	505	LEU	2.0
1	A	556	LYS	2.0
1	B	527	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

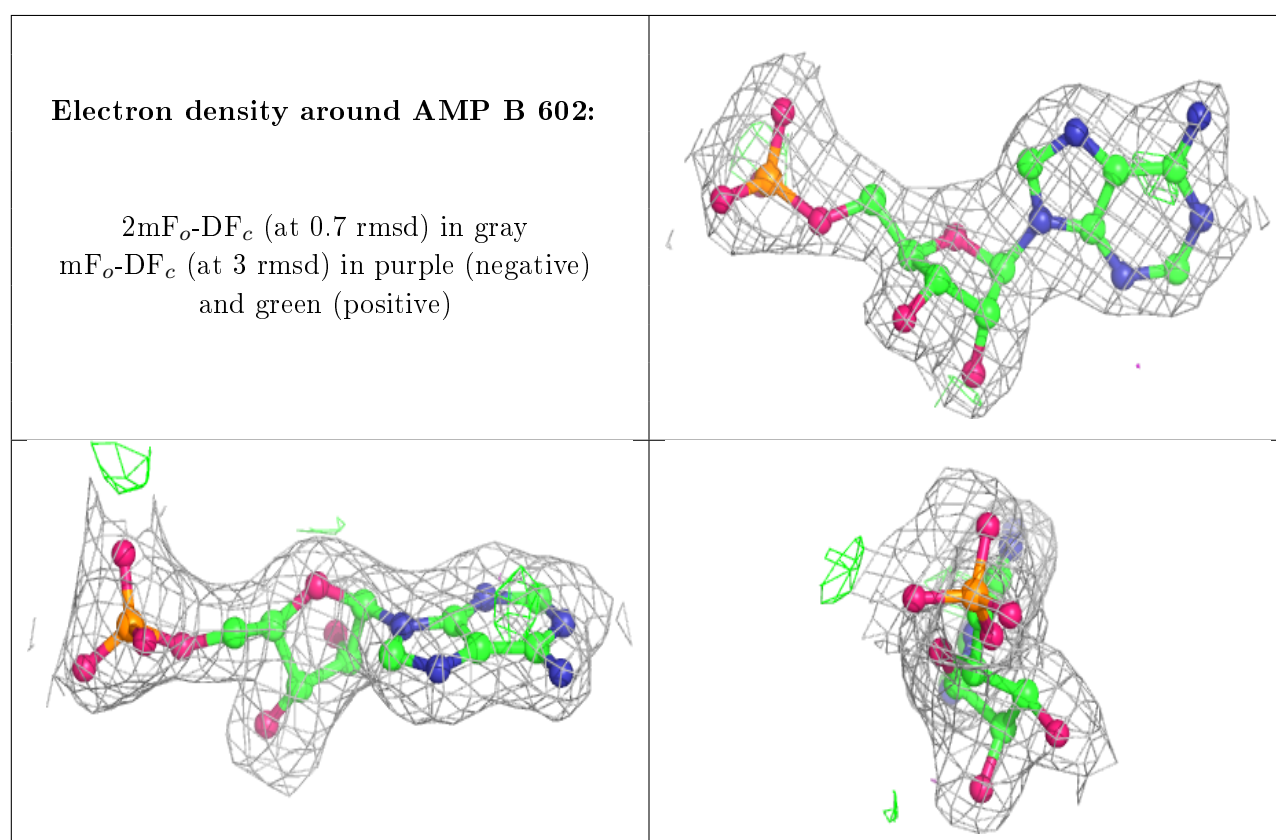
## 6.4 Ligands [i](#)

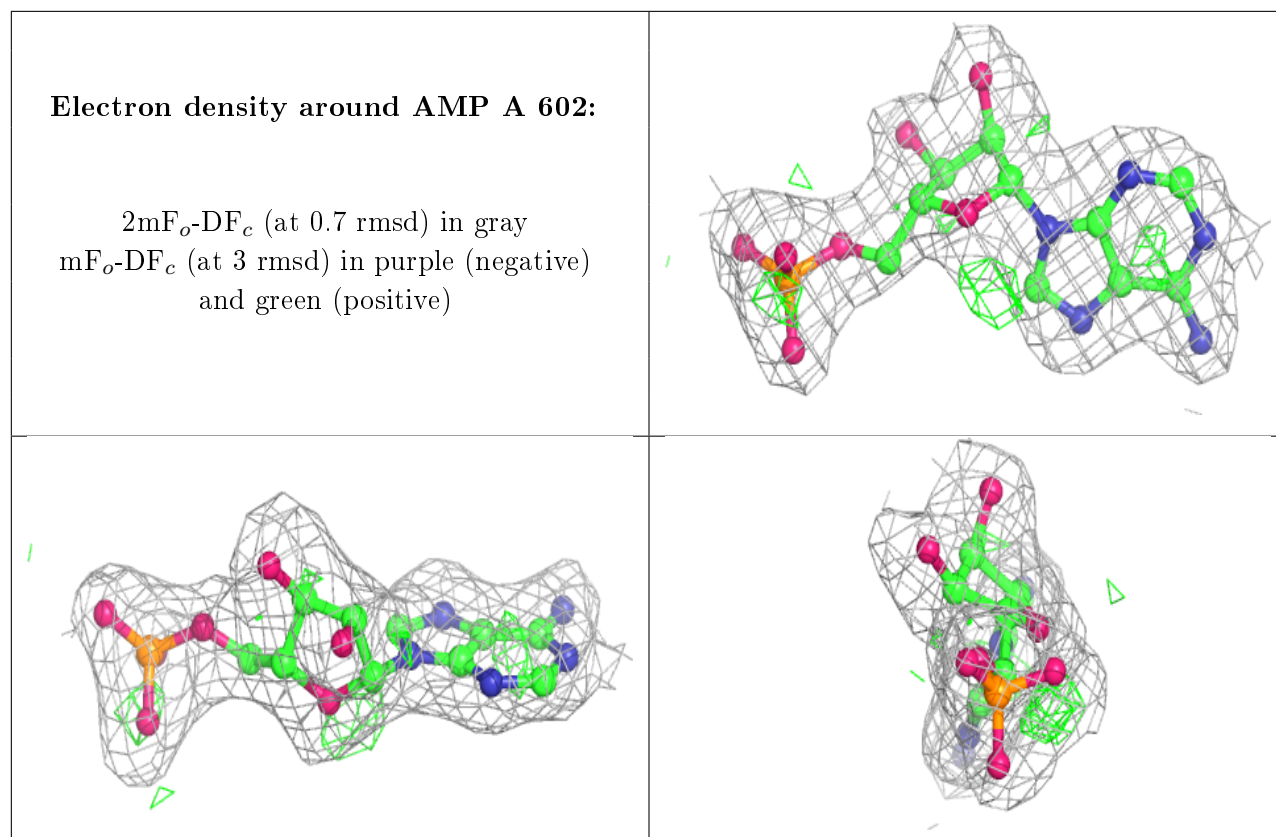
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	SAL	B	601	10/10	0.91	0.15	19,26,29,31	0
3	AMP	B	602	23/23	0.94	0.11	12,22,30,36	0
2	SAL	A	601	10/10	0.95	0.12	18,24,26,28	0
3	AMP	A	602	23/23	0.96	0.12	10,21,32,36	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.