



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 05:45 AM EDT

PDB ID : 2RHQ  
Title : PheRS from Staphylococcus haemolyticus- rational protein engineering and inhibitor studies  
Authors : Evdokimov, A.G.; Mekel, M.  
Deposited on : 2007-10-09  
Resolution : 2.20 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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.23.2  
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) : 2.23.2

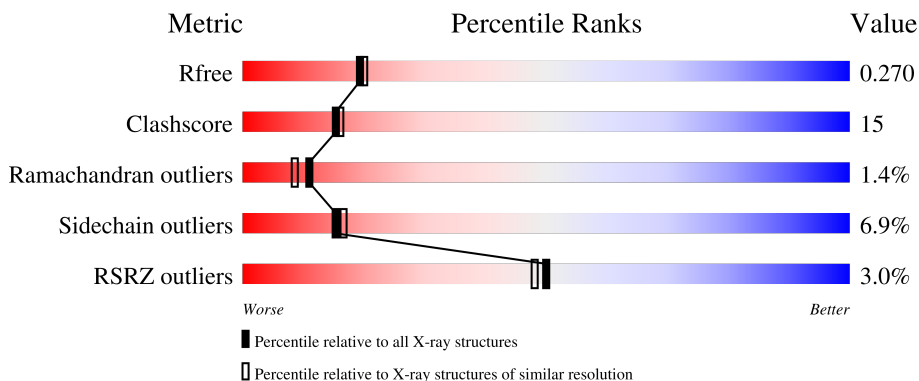
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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	294	 3% 67% 22% 8%
2	B	795	 3% 69% 26% 2%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 8715 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 Phenylalanyl-tRNA synthetase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	270	2176	1377	366	418	15	0	4	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	58	MET	-	expression tag	UNP Q4L5E3
A	59	GLY	-	expression tag	UNP Q4L5E3
A	60	SER	-	expression tag	UNP Q4L5E3
A	61	SER	-	expression tag	UNP Q4L5E3
A	62	HIS	-	expression tag	UNP Q4L5E3
A	63	HIS	-	expression tag	UNP Q4L5E3
A	64	HIS	-	expression tag	UNP Q4L5E3
A	65	HIS	-	expression tag	UNP Q4L5E3
A	66	HIS	-	expression tag	UNP Q4L5E3
A	67	HIS	-	expression tag	UNP Q4L5E3
A	68	SER	-	expression tag	UNP Q4L5E3
A	69	SER	-	expression tag	UNP Q4L5E3
A	70	GLY	-	expression tag	UNP Q4L5E3
A	71	LEU	-	expression tag	UNP Q4L5E3
A	72	VAL	-	expression tag	UNP Q4L5E3
A	73	PRO	-	expression tag	UNP Q4L5E3
A	74	ARG	-	expression tag	UNP Q4L5E3
A	75	GLY	-	expression tag	UNP Q4L5E3
A	76	SER	-	expression tag	UNP Q4L5E3
A	77	HIS	-	expression tag	UNP Q4L5E3
A	78	MET	-	expression tag	UNP Q4L5E3
A	79	GLY	-	expression tag	UNP Q4L5E3
A	80	THR	-	expression tag	UNP Q4L5E3
A	81	GLU	-	expression tag	UNP Q4L5E3
A	82	LEU	-	expression tag	UNP Q4L5E3
A	83	MET	-	expression tag	UNP Q4L5E3

- Molecule 2 is a protein called Phenylalanyl-tRNA synthetase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	790	6159	3871	1039	1232	17	0	0	0

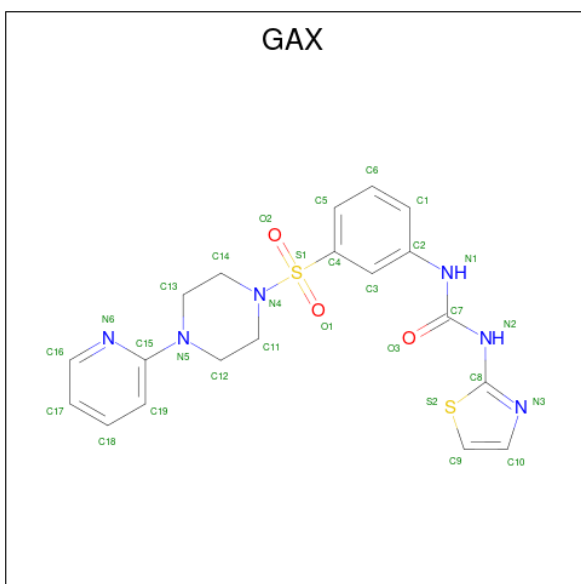
There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	34	ASN	ASP	engineered mutation	UNP Q4L5E4
B	?	-	HIS	deletion	UNP Q4L5E4
B	?	-	PRO	deletion	UNP Q4L5E4
B	56	GLY	ASP	engineered mutation	UNP Q4L5E4
B	57	SER	ALA	engineered mutation	UNP Q4L5E4
B	62	GLY	ASP	engineered mutation	UNP Q4L5E4
B	?	-	LYS	deletion	UNP Q4L5E4
B	?	-	LEU	deletion	UNP Q4L5E4
B	144	PRO	GLN	engineered mutation	UNP Q4L5E4
B	795	GLU	GLN	engineered mutation	UNP Q4L5E4

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 1-{3-[(4-pyridin-2-ylpiperazin-1-yl)sulfonyl]phenyl}-3-(1,3-thiazol-2-yl)urea (three-letter code: GAX) (formula: C<sub>19</sub>H<sub>20</sub>N<sub>6</sub>O<sub>3</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	30	19	6	3	2	0	0

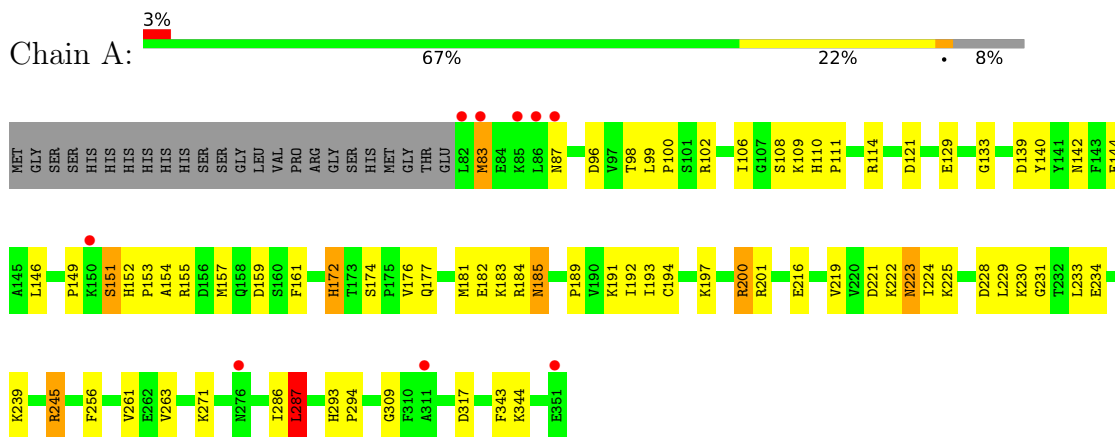
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	87	Total 87	O 87	0	0
5	B	262	Total 262	O 262	0	0

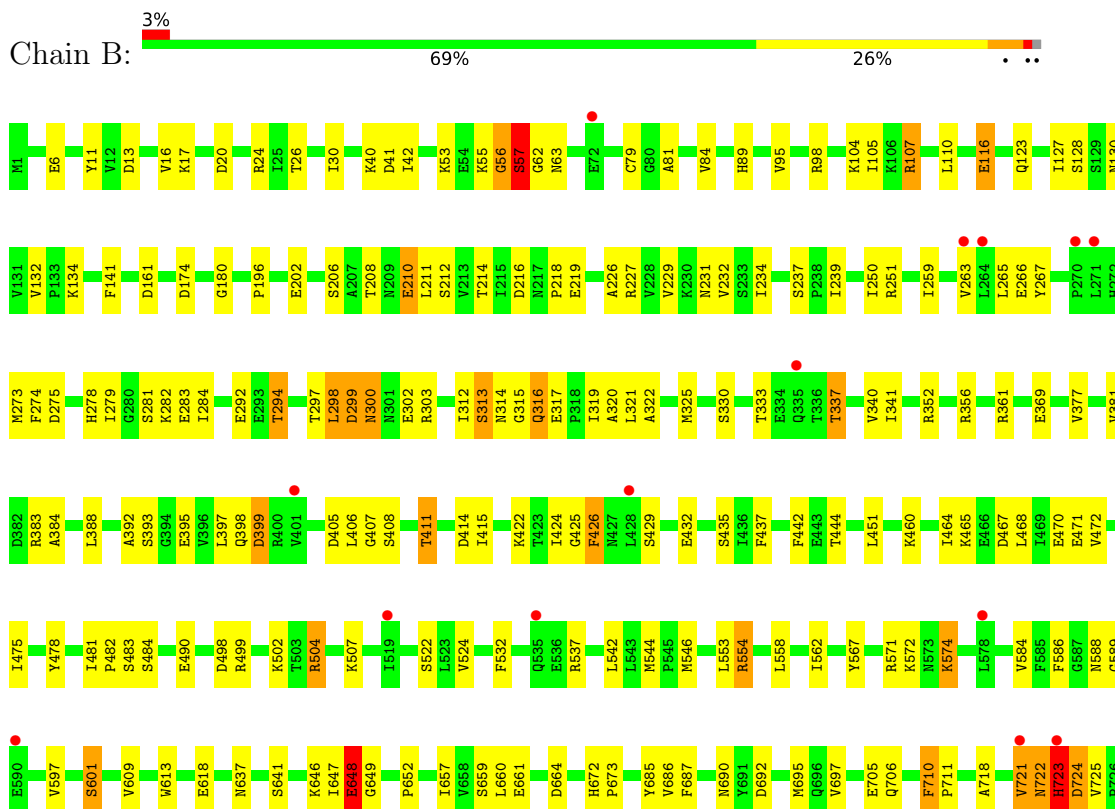
### 3 Residue-property plots i

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: Phenylalanyl-tRNA synthetase alpha chain



- Molecule 2: Phenylalanyl-tRNA synthetase beta chain





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	249.31Å 87.60Å 61.07Å 90.00° 100.44° 90.00°	Depositor
Resolution (Å)	35.60 – 2.20 32.52 – 2.20	Depositor EDS
% Data completeness (in resolution range)	95.7 (35.60-2.20) 95.7 (32.52-2.20)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.20Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.196 , 0.269 0.202 , 0.270	Depositor DCC
$R_{free}$ test set	3192 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.6	Xtrriage
Anisotropy	0.178	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 54.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8715	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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: ZN, GAX

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	0.74	0/2233	0.80	1/3012 (0.0%)
2	B	0.76	0/6254	0.77	2/8474 (0.0%)
All	All	0.76	0/8487	0.78	3/11486 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	18
All	All	0	20

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	504	ARG	NE-CZ-NH1	7.67	124.14	120.30
2	B	504	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	A	102	ARG	NE-CZ-NH1	-5.08	117.76	120.30

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	SER	Peptide
1	A	287	LEU	Peptide
2	B	210	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	B	294	THR	Peptide
2	B	298	LEU	Peptide
2	B	299	ASP	Peptide
2	B	315	GLY	Peptide
2	B	316	GLN	Peptide
2	B	407	GLY	Peptide
2	B	553	LEU	Peptide
2	B	56	GLY	Peptide
2	B	57	SER	Peptide
2	B	589	GLY	Peptide
2	B	647	ILE	Peptide
2	B	721	VAL	Peptide
2	B	723	HIS	Peptide
2	B	740	ASP	Peptide
2	B	751	TYR	Peptide
2	B	795	GLU	Peptide
2	B	798	THR	Peptide

## 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	2176	0	2133	58	0
2	B	6159	0	6132	200	0
3	A	1	0	0	0	0
4	A	30	0	20	1	0
5	A	87	0	0	7	0
5	B	262	0	0	17	0
All	All	8715	0	8285	248	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 15.

All (248) 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)
2:B:733:ILE:CD1	2:B:792:LEU:HD23	1.68	1.24
2:B:733:ILE:HD11	2:B:792:LEU:CD2	1.72	1.20
2:B:648:GLU:HG3	2:B:649:GLY:N	1.43	1.13
2:B:411:THR:HG23	5:B:1038:HOH:O	1.55	1.04
2:B:722:ASN:HB2	2:B:725:VAL:HG23	1.51	0.93
2:B:107:ARG:HH21	2:B:107:ARG:HG3	1.34	0.92
2:B:17:LYS:HD3	5:B:1056:HOH:O	1.68	0.92
2:B:648:GLU:CG	2:B:649:GLY:N	2.30	0.91
2:B:648:GLU:HG3	2:B:649:GLY:H	1.15	0.91
2:B:98:ARG:CZ	2:B:104:LYS:HG2	2.01	0.90
2:B:737:ASN:OD1	2:B:791:ALA:HB2	1.71	0.90
2:B:725:VAL:O	2:B:761:LYS:NZ	2.05	0.89
2:B:17:LYS:HB3	5:B:1056:HOH:O	1.73	0.88
2:B:798:THR:HG22	2:B:799:ILE:H	1.37	0.88
2:B:210:GLU:O	2:B:282:LYS:HG2	1.74	0.87
2:B:785:HIS:O	2:B:789:LEU:HD12	1.74	0.87
2:B:499:ARG:HG3	2:B:695:MET:HE3	1.58	0.85
2:B:648:GLU:CG	2:B:649:GLY:H	1.89	0.85
2:B:107:ARG:HH22	2:B:116:GLU:CG	1.91	0.83
2:B:297:THR:O	2:B:299:ASP:N	2.12	0.82
2:B:721:VAL:CG1	2:B:725:VAL:HB	2.10	0.81
2:B:107:ARG:HH22	2:B:116:GLU:HG2	1.46	0.80
2:B:722:ASN:CB	2:B:725:VAL:HG23	2.13	0.79
2:B:206:SER:OG	2:B:399:ASP:OD2	1.99	0.79
2:B:415:ILE:HD12	2:B:465:LYS:HB2	1.62	0.79
1:A:106:ILE:O	1:A:344:LYS:HE2	1.82	0.79
1:A:109:LYS:HG3	5:B:1041:HOH:O	1.82	0.79
2:B:776:LEU:HD11	2:B:781:VAL:CG2	2.13	0.79
2:B:722:ASN:HB2	2:B:725:VAL:CG2	2.13	0.77
2:B:721:VAL:HG11	2:B:725:VAL:HB	1.66	0.75
1:A:225:LYS:HE2	5:A:434:HOH:O	1.85	0.75
2:B:107:ARG:HG3	2:B:107:ARG:NH2	1.94	0.75
2:B:499:ARG:HG3	2:B:695:MET:CE	2.16	0.75
2:B:721:VAL:HG12	2:B:722:ASN:O	1.87	0.74
2:B:532:PHE:CD1	2:B:648:GLU:HG2	2.22	0.74
2:B:499:ARG:HA	2:B:695:MET:CE	2.20	0.72
1:A:154:ALA:O	5:A:382:HOH:O	2.07	0.72
1:A:234:GLU:OE1	2:B:483:SER:OG	2.08	0.71
1:A:96:ASP:OD1	1:A:98[A]:THR:OG1	2.08	0.70
2:B:63:ASN:HB2	2:B:79:CYS:O	1.91	0.70
2:B:798:THR:HG22	2:B:799:ILE:N	2.06	0.70
2:B:405:ASP:OD2	2:B:406:LEU:O	2.08	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ARG:HD2	5:A:373:HOH:O	1.90	0.69
1:A:189:PRO:HG3	5:B:995:HOH:O	1.92	0.69
2:B:279:ILE:HD11	2:B:340:VAL:HG11	1.74	0.69
2:B:737:ASN:OD1	2:B:791:ALA:CB	2.41	0.68
2:B:98:ARG:NH2	2:B:104:LYS:HG2	2.09	0.67
2:B:723:HIS:CD2	2:B:723:HIS:O	2.48	0.67
2:B:637:ASN:ND2	5:B:905:HOH:O	2.09	0.67
2:B:107:ARG:HH21	2:B:107:ARG:CG	2.06	0.66
2:B:733:ILE:HG13	2:B:734:ILE:H	1.61	0.66
2:B:735:HIS:NE2	2:B:745:THR:HG22	2.11	0.66
2:B:574:LYS:HD2	5:B:1047:HOH:O	1.96	0.65
1:A:230:LYS:NZ	2:B:481:ILE:O	2.27	0.64
2:B:234:ILE:CD1	2:B:333:THR:O	2.46	0.63
5:A:357:HOH:O	2:B:504:ARG:HD2	1.98	0.63
2:B:723:HIS:ND1	2:B:752:GLU:OE1	2.32	0.63
1:A:159:ASP:HB3	1:A:200:ARG:HH22	1.64	0.62
1:A:174:SER:OG	1:A:216:GLU:OE1	2.17	0.62
1:A:200:ARG:HB2	5:A:411:HOH:O	1.99	0.62
2:B:731:LYS:HE3	2:B:745:THR:HG23	1.82	0.61
1:A:83:MET:O	1:A:87:ASN:ND2	2.33	0.61
2:B:16:VAL:CG1	2:B:20:ASP:HB2	2.31	0.61
2:B:733:ILE:HG13	2:B:734:ILE:N	2.16	0.61
2:B:40:LYS:O	2:B:41:ASP:HB2	2.00	0.60
2:B:723:HIS:O	2:B:723:HIS:CG	2.54	0.60
2:B:352:ARG:HB2	2:B:369:GLU:HG2	1.84	0.60
2:B:785:HIS:CD2	2:B:789:LEU:HD11	2.36	0.59
1:A:140:TYR:HA	1:A:144[A]:GLU:HB2	1.84	0.59
2:B:279:ILE:HD11	2:B:340:VAL:CG1	2.31	0.59
1:A:161:PHE:CD1	2:B:542:LEU:HD13	2.37	0.59
2:B:174:ASP:O	2:B:180:GLY:HA3	2.03	0.59
1:A:231:GLY:HA3	2:B:484:SER:O	2.03	0.59
2:B:426:PHE:CE2	2:B:481:ILE:HD13	2.39	0.58
2:B:731:LYS:CE	2:B:745:THR:HG23	2.34	0.58
2:B:499:ARG:CG	2:B:695:MET:HE3	2.33	0.57
2:B:464:ILE:O	2:B:467:ASP:HB2	2.03	0.57
1:A:144[A]:GLU:HG2	1:A:155:ARG:HH12	1.68	0.57
1:A:223:ASN:O	1:A:225:LYS:NZ	2.35	0.56
2:B:733:ILE:HD12	2:B:792:LEU:HA	1.87	0.56
2:B:429:SER:N	2:B:432:GLU:OE2	2.26	0.56
2:B:788:ILE:HG22	2:B:789:LEU:N	2.21	0.56
2:B:297:THR:C	2:B:299:ASP:N	2.57	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:LEU:CD1	1:A:172:HIS:CE1	2.88	0.56
2:B:411:THR:CG2	5:B:1038:HOH:O	2.30	0.56
1:A:197:LYS:HE2	5:B:926:HOH:O	2.05	0.56
2:B:733:ILE:HD11	2:B:792:LEU:HD23	0.75	0.55
2:B:89:HIS:HE1	5:B:1055:HOH:O	1.88	0.55
2:B:733:ILE:CD1	2:B:792:LEU:HA	2.37	0.55
1:A:317:ASP:HB2	5:A:433:HOH:O	2.07	0.55
2:B:499:ARG:CG	2:B:695:MET:CE	2.84	0.55
2:B:724:ASP:OD1	2:B:724:ASP:O	2.24	0.55
2:B:98:ARG:NE	2:B:104:LYS:HG2	2.22	0.55
1:A:144[A]:GLU:OE1	1:A:149:PRO:HA	2.07	0.54
2:B:250:ILE:HD12	2:B:265:LEU:HD11	1.88	0.54
2:B:584:VAL:CG2	2:B:597:VAL:HG13	2.38	0.54
2:B:499:ARG:HA	2:B:695:MET:HE3	1.88	0.53
1:A:109:LYS:HE2	5:B:1037:HOH:O	2.07	0.53
1:A:201:ARG:CZ	2:B:544:MET:HE2	2.39	0.53
2:B:274:PHE:HB2	2:B:340:VAL:CG1	2.38	0.53
2:B:411:THR:O	2:B:411:THR:OG1	2.26	0.53
1:A:140:TYR:CD1	1:A:144[B]:GLU:HB3	2.44	0.53
2:B:281:SER:OG	2:B:314:ASN:HB2	2.09	0.53
2:B:498:ASP:O	2:B:502:LYS:HG3	2.08	0.53
2:B:502:LYS:HB2	2:B:695:MET:HE1	1.90	0.53
2:B:226:ALA:HA	2:B:341:ILE:O	2.09	0.52
2:B:584:VAL:HG22	2:B:597:VAL:HG13	1.91	0.52
2:B:690:ASN:OD1	2:B:692:ASP:HB2	2.08	0.52
2:B:558:LEU:O	2:B:562:ILE:HG13	2.09	0.52
1:A:139:ASP:OD1	1:A:155:ARG:NH2	2.43	0.52
2:B:55:LYS:HA	2:B:62:GLY:O	2.11	0.51
2:B:657:ILE:HG21	2:B:664:ASP:OD1	2.09	0.51
2:B:798:THR:CG2	2:B:799:ILE:N	2.71	0.51
2:B:274:PHE:HD1	2:B:330:SER:HB2	1.76	0.51
2:B:524:VAL:HG22	2:B:554:ARG:H	1.75	0.51
1:A:201:ARG:HG2	2:B:546:MET:CE	2.41	0.51
2:B:42:ILE:HA	2:B:98:ARG:O	2.11	0.50
2:B:722:ASN:HB3	2:B:724:ASP:HB3	1.93	0.50
2:B:730:LEU:O	2:B:731:LYS:C	2.48	0.50
2:B:231:ASN:ND2	2:B:395:GLU:OE2	2.28	0.50
2:B:567:TYR:CE1	2:B:571:ARG:NH1	2.80	0.50
2:B:782:SER:O	2:B:786:ASP:OD2	2.29	0.50
2:B:723:HIS:HA	2:B:761:LYS:HD3	1.93	0.50
1:A:146:LEU:HD13	1:A:172:HIS:CE1	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:352:GAX:O3	4:A:352:GAX:S2	2.70	0.50
2:B:398:GLN:O	2:B:399:ASP:HB2	2.12	0.50
2:B:424:ILE:CG2	2:B:481:ILE:HD12	2.41	0.50
2:B:537:ARG:HG2	2:B:586:PHE:CD1	2.46	0.49
2:B:6:GLU:HB2	2:B:161:ASP:OD1	2.12	0.49
2:B:16:VAL:HG12	2:B:17:LYS:O	2.11	0.49
2:B:26:THR:HA	2:B:30:ILE:O	2.11	0.49
2:B:532:PHE:CE1	2:B:648:GLU:HG2	2.47	0.49
2:B:259:ILE:O	2:B:263:VAL:HG23	2.13	0.49
2:B:377:VAL:O	2:B:381:VAL:HG23	2.12	0.49
2:B:537:ARG:HG2	2:B:586:PHE:HB3	1.93	0.49
2:B:710:PHE:HB3	2:B:711:PRO:HD2	1.94	0.49
1:A:201:ARG:HG2	2:B:546:MET:HE2	1.94	0.48
2:B:737:ASN:N	2:B:737:ASN:HD22	2.10	0.48
1:A:177:GLN:HG2	1:A:194[A]:CYS:SG	2.53	0.48
1:A:230:LYS:O	1:A:234:GLU:HG3	2.13	0.48
2:B:522:SER:O	2:B:554:ARG:HB2	2.12	0.48
2:B:107:ARG:NH2	2:B:116:GLU:HG2	2.23	0.48
1:A:200:ARG:HG3	1:A:200:ARG:HH21	1.78	0.48
2:B:211:LEU:HD11	2:B:284:ILE:HD12	1.94	0.48
1:A:96:ASP:CG	1:A:98[A]:THR:HG1	2.13	0.48
2:B:210:GLU:HG3	2:B:397:LEU:CD2	2.42	0.48
2:B:785:HIS:O	2:B:788:ILE:HB	2.13	0.48
2:B:196:PRO:HD2	2:B:267:TYR:OH	2.12	0.48
1:A:201:ARG:CZ	2:B:544:MET:CE	2.92	0.48
2:B:499:ARG:HA	2:B:695:MET:HE1	1.94	0.48
2:B:275:ASP:HB3	2:B:278:HIS:HB2	1.95	0.47
2:B:741:ILE:HD11	2:B:784:ILE:HD12	1.96	0.47
1:A:229:LEU:O	1:A:233:LEU:HG	2.14	0.47
2:B:478:TYR:HA	2:B:481:ILE:HG12	1.96	0.47
2:B:706:GLN:O	2:B:772:THR:HG21	2.13	0.47
2:B:786:ASP:HA	2:B:789:LEU:HD13	1.96	0.47
2:B:202:GLU:OE2	2:B:227:ARG:NH2	2.37	0.47
2:B:274:PHE:HB2	2:B:340:VAL:HG13	1.95	0.47
2:B:299:ASP:OD2	2:B:303:ARG:NH2	2.47	0.47
2:B:11:TYR:OH	2:B:266:GLU:HG3	2.14	0.47
2:B:141:PHE:HZ	2:B:239:ILE:HD13	1.80	0.47
2:B:609:VAL:HB	2:B:618:GLU:HB3	1.97	0.47
2:B:776:LEU:HD11	2:B:781:VAL:HG22	1.95	0.47
2:B:571:ARG:O	2:B:572:LYS:HB2	2.14	0.47
2:B:672:HIS:ND1	2:B:673:PRO:HD2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:TYR:HA	1:A:144[B]:GLU:HB2	1.97	0.46
2:B:297:THR:HB	2:B:325:MET:SD	2.55	0.46
2:B:425:GLY:O	2:B:482:PRO:HG2	2.16	0.46
2:B:718:ALA:O	2:B:799:ILE:HB	2.16	0.46
2:B:468:LEU:O	2:B:472:VAL:HG23	2.16	0.46
2:B:742:LEU:HD13	2:B:767:LEU:HD23	1.98	0.46
1:A:142:ASN:O	1:A:146:LEU:HD12	2.16	0.45
1:A:228:ASP:OD2	2:B:484:SER:OG	2.32	0.45
2:B:437:PHE:O	2:B:442:PHE:HB2	2.16	0.45
2:B:601:SER:HB3	2:B:687:PHE:O	2.17	0.45
1:A:263:VAL:HB	1:A:287:LEU:HB2	1.99	0.45
2:B:471:GLU:O	2:B:475:ILE:HG12	2.17	0.45
1:A:110:HIS:O	1:A:114:ARG:HG3	2.16	0.45
2:B:721:VAL:CG1	2:B:725:VAL:CB	2.90	0.45
2:B:746:LEU:O	2:B:765:ILE:HA	2.17	0.45
1:A:96:ASP:OD1	1:A:98[A]:THR:HG23	2.17	0.45
2:B:444:THR:CG2	2:B:451:LEU:HD22	2.45	0.45
2:B:312:ILE:CD1	2:B:322:ALA:HB2	2.47	0.45
2:B:652:PRO:HA	5:B:810:HOH:O	2.15	0.45
1:A:221:ASP:HB3	1:A:224:ILE:HG12	1.99	0.44
2:B:107:ARG:HH22	2:B:116:GLU:HG3	1.78	0.44
2:B:352:ARG:HG2	2:B:356:ARG:HD3	1.99	0.44
2:B:16:VAL:HG13	2:B:20:ASP:HB2	1.99	0.44
2:B:210:GLU:O	2:B:282:LYS:CG	2.57	0.44
2:B:313:SER:OG	2:B:314:ASN:N	2.49	0.44
1:A:108[B]:SER:OG	1:A:343:PHE:C	2.56	0.44
2:B:742:LEU:CD1	2:B:767:LEU:HD23	2.47	0.44
2:B:319:ILE:O	2:B:320:ALA:HB2	2.17	0.44
1:A:96:ASP:OD1	1:A:98[A]:THR:CG2	2.66	0.44
2:B:648:GLU:HG3	2:B:649:GLY:CA	2.37	0.44
2:B:294:THR:CG2	5:B:1059:HOH:O	2.65	0.44
2:B:123:GLN:HA	2:B:127:ILE:O	2.19	0.43
2:B:128:SER:OG	2:B:130:ASN:HB2	2.18	0.43
2:B:558:LEU:HD13	2:B:686:VAL:HG21	2.00	0.43
1:A:152:HIS:ND1	1:A:153:PRO:HD2	2.34	0.43
2:B:206:SER:OG	2:B:208:THR:HG23	2.19	0.43
1:A:245:ARG:HA	1:A:245:ARG:HD3	1.87	0.43
2:B:132:VAL:O	2:B:251:ARG:NH1	2.46	0.43
1:A:200:ARG:HG3	1:A:200:ARG:NH2	2.34	0.43
2:B:81:ALA:O	2:B:84:VAL:HG12	2.18	0.43
1:A:100:PRO:HD2	2:B:613:TRP:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:743:GLN:HB3	2:B:768:ASN:O	2.19	0.43
2:B:723:HIS:HB2	2:B:761:LYS:HB3	1.99	0.43
2:B:733:ILE:CG1	2:B:734:ILE:H	2.30	0.42
2:B:229:VAL:HG13	2:B:341:ILE:HD11	2.00	0.42
1:A:121:ASP:CG	2:B:504:ARG:HH22	2.22	0.42
2:B:53:LYS:HE3	2:B:63:ASN:OD1	2.19	0.42
1:A:109:LYS:CE	5:B:1037:HOH:O	2.66	0.42
2:B:56:GLY:O	2:B:57:SER:HB2	2.18	0.42
2:B:660:LEU:HG	2:B:661:GLU:HG3	2.01	0.42
2:B:722:ASN:O	2:B:725:VAL:N	2.51	0.42
1:A:111:PRO:HD3	5:A:369:HOH:O	2.19	0.42
2:B:444:THR:HG22	2:B:451:LEU:HD22	2.01	0.42
2:B:279:ILE:O	2:B:314:ASN:ND2	2.52	0.42
1:A:192:ILE:O	1:A:193:ILE:HD13	2.20	0.42
2:B:384:ALA:O	2:B:388:LEU:HG	2.19	0.42
1:A:133:GLY:HA3	1:A:176:VAL:HG22	2.01	0.41
2:B:426:PHE:CE2	2:B:481:ILE:CD1	3.02	0.41
2:B:337:THR:HG22	5:B:1051:HOH:O	2.20	0.41
2:B:107:ARG:NH2	2:B:116:GLU:CG	2.72	0.41
2:B:722:ASN:C	2:B:724:ASP:HB3	2.41	0.41
2:B:95:VAL:HA	2:B:105:ILE:HG22	2.02	0.41
2:B:294:THR:HG23	2:B:302:GLU:HG3	2.03	0.41
2:B:426:PHE:HD2	2:B:426:PHE:HA	1.77	0.41
1:A:219:VAL:O	1:A:309:GLY:HA2	2.20	0.41
1:A:225:LYS:O	1:A:228:ASP:HB2	2.21	0.41
2:B:134:LYS:HA	2:B:134:LYS:HD3	1.87	0.41
2:B:507:LYS:HE2	5:B:1041:HOH:O	2.21	0.41
2:B:537:ARG:HG2	2:B:586:PHE:HD1	1.86	0.41
2:B:733:ILE:CG1	2:B:734:ILE:N	2.84	0.41
1:A:286:ILE:HD12	1:A:287:LEU:HD12	2.03	0.41
2:B:685:TYR:CD2	2:B:685:TYR:N	2.89	0.41
2:B:216:ASP:C	2:B:218:PRO:HD3	2.40	0.40
2:B:426:PHE:CZ	2:B:481:ILE:CD1	3.04	0.40
2:B:588:ASN:N	5:B:934:HOH:O	2.53	0.40
2:B:737:ASN:O	2:B:787:LYS:NZ	2.51	0.40
2:B:781:VAL:O	2:B:785:HIS:HB2	2.21	0.40
2:B:499:ARG:CG	2:B:695:MET:HE2	2.51	0.40
2:B:567:TYR:O	2:B:571:ARG:HG2	2.21	0.40
1:A:99:LEU:HA	1:A:100:PRO:HD3	1.88	0.40
2:B:232:VAL:HA	2:B:392:ALA:O	2.21	0.40
2:B:740:ASP:HB3	2:B:741:ILE:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:HIS:HA	1:A:294:PRO:HD2	1.82	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	272/294 (92%)	250 (92%)	19 (7%)	3 (1%)	14	12
2	B	786/795 (99%)	724 (92%)	50 (6%)	12 (2%)	10	8
All	All	1058/1089 (97%)	974 (92%)	69 (6%)	15 (1%)	11	8

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	185	ASN
2	B	57	SER
2	B	298	LEU
2	B	554	ARG
2	B	724	ASP
2	B	300	ASN
2	B	648	GLU
1	A	271	LYS
2	B	399	ASP
2	B	727	SER
1	A	183	LYS
2	B	722	ASN
2	B	316	GLN
2	B	734	ILE
2	B	697	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	241/257 (94%)	224 (93%)	17 (7%)	14	16
2	B	681/685 (99%)	635 (93%)	46 (7%)	16	17
All	All	922/942 (98%)	859 (93%)	63 (7%)	15	17

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	MET
1	A	129	GLU
1	A	151	SER
1	A	157	MET
1	A	172	HIS
1	A	181	MET
1	A	182	GLU
1	A	185	ASN
1	A	191	LYS
1	A	200	ARG
1	A	222	LYS
1	A	223	ASN
1	A	239	LYS
1	A	245	ARG
1	A	256	PHE
1	A	261	VAL
1	A	287	LEU
2	B	13	ASP
2	B	24	ARG
2	B	57	SER
2	B	107	ARG
2	B	110	LEU
2	B	116	GLU
2	B	212	SER
2	B	214	THR
2	B	219	GLU
2	B	237	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	273	MET
2	B	283	GLU
2	B	292	GLU
2	B	300	ASN
2	B	313	SER
2	B	317	GLU
2	B	321	LEU
2	B	337	THR
2	B	361	ARG
2	B	383	ARG
2	B	393	SER
2	B	408	SER
2	B	411	THR
2	B	414	ASP
2	B	422	LYS
2	B	426	PHE
2	B	435	SER
2	B	460	LYS
2	B	470	GLU
2	B	490	GLU
2	B	574	LYS
2	B	601	SER
2	B	641	SER
2	B	646	LYS
2	B	648	GLU
2	B	659	SER
2	B	705	GLU
2	B	710	PHE
2	B	723	HIS
2	B	736	ASN
2	B	737	ASN
2	B	740	ASP
2	B	751	TYR
2	B	752	GLU
2	B	780	ARG
2	B	787	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GAX	A	352	-	31,33,33	1.52	3 (9%)	38,46,46	3.02	20 (52%)

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
4	GAX	A	352	-	-	6/22/34/34	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	352	GAX	C4-S1	-6.15	1.67	1.76
4	A	352	GAX	C2-N1	-2.83	1.35	1.41
4	A	352	GAX	C15-N5	2.73	1.43	1.37

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	352	GAX	O2-S1-C4	8.41	118.68	108.05
4	A	352	GAX	O2-S1-O1	-7.29	107.70	119.52
4	A	352	GAX	C2-C3-C4	5.27	122.86	118.89
4	A	352	GAX	C5-C4-C3	-5.04	114.43	120.62
4	A	352	GAX	C4-S1-N4	-4.53	101.91	107.30
4	A	352	GAX	C12-N5-C15	-4.33	110.34	120.39
4	A	352	GAX	C6-C5-C4	4.01	123.11	118.95
4	A	352	GAX	C13-N5-C15	-3.52	112.22	120.39
4	A	352	GAX	C16-N6-C15	3.39	121.34	116.86
4	A	352	GAX	O1-S1-N4	3.31	109.71	106.69
4	A	352	GAX	C3-C4-S1	3.09	122.78	119.34
4	A	352	GAX	C5-C4-S1	2.83	122.74	119.76
4	A	352	GAX	C13-C14-N4	2.70	110.98	108.91
4	A	352	GAX	C19-C15-N6	-2.61	118.62	123.41
4	A	352	GAX	O1-S1-C4	2.53	111.24	108.05
4	A	352	GAX	C18-C19-C15	2.33	120.82	117.66
4	A	352	GAX	C14-C13-N5	2.12	114.82	110.70
4	A	352	GAX	C12-C11-N4	-2.10	107.31	108.91
4	A	352	GAX	N6-C15-N5	2.04	119.84	116.79
4	A	352	GAX	N2-C7-N1	2.01	116.01	112.49

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	352	GAX	C11-N4-S1-O2
4	A	352	GAX	C14-N4-S1-O1
4	A	352	GAX	C11-N4-S1-O1
4	A	352	GAX	C11-N4-S1-C4
4	A	352	GAX	C14-N4-S1-C4
4	A	352	GAX	C14-N4-S1-O2

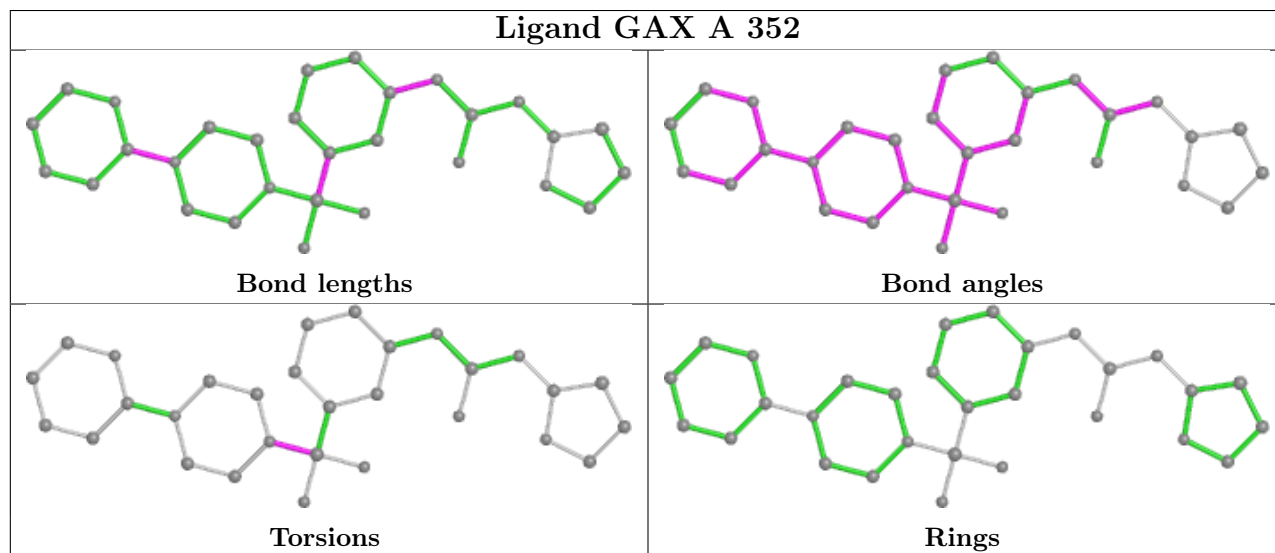
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	352	GAX	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	270/294 (91%)	0.03	9 (3%) 46 44	30, 44, 71, 107	0
2	B	790/795 (99%)	-0.02	23 (2%) 51 49	27, 48, 69, 99	0
All	All	1060/1089 (97%)	-0.01	32 (3%) 50 48	27, 47, 69, 107	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	83	MET	5.0
2	B	751	TYR	4.9
1	A	351	GLU	4.0
1	A	85	LYS	3.5
1	A	87	ASN	3.3
2	B	578	LEU	3.2
1	A	82	LEU	3.0
2	B	264	LEU	3.0
1	A	311	ALA	2.9
2	B	590	GLU	2.9
2	B	797	ALA	2.8
2	B	271	LEU	2.7
2	B	723	HIS	2.6
2	B	721	VAL	2.6
2	B	788	ILE	2.5
2	B	263	VAL	2.5
1	A	86	LEU	2.5
2	B	760	LYS	2.4
2	B	535	GLN	2.4
2	B	790	GLU	2.4
2	B	519	ILE	2.4
2	B	774	ASP	2.4
2	B	401	VAL	2.4
2	B	335	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	72	GLU	2.2
2	B	428	LEU	2.2
2	B	758	LYS	2.2
1	A	150	LYS	2.1
2	B	792	LEU	2.1
1	A	276	ASN	2.1
2	B	270	PRO	2.1
2	B	752	GLU	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.

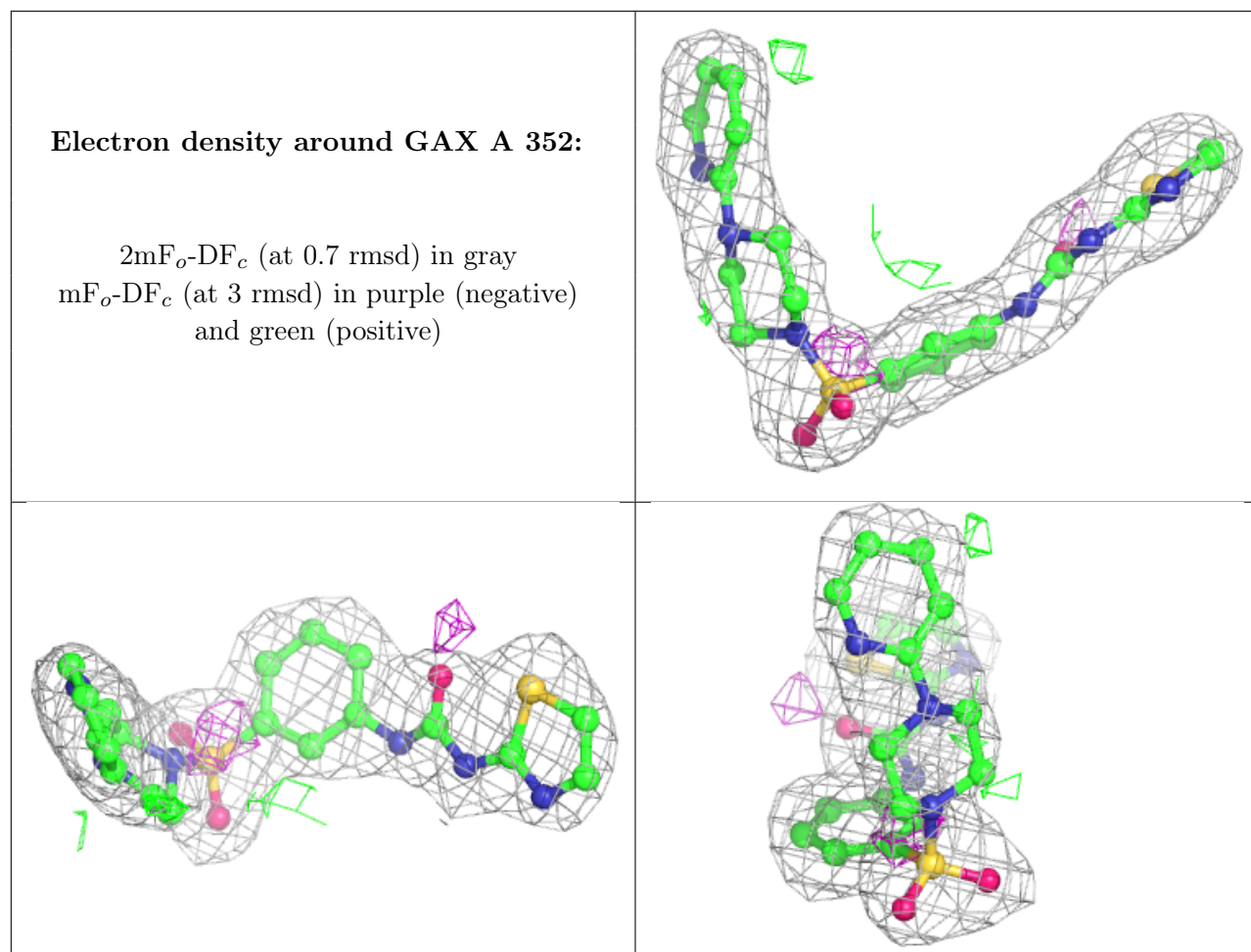
## 6.4 Ligands [i](#)

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, 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
4	GAX	A	352	30/30	0.97	0.11	29,46,66,67	0
3	ZN	A	1	1/1	0.98	0.07	57,57,57,57	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.