

Full wwPDB X-ray Structure Validation Report (i)

Feb 21, 2022 – 06:21 pm GMT

PDB ID	:	7BIC
Title	:	Crystal structure of human GSTA1-1 bound to allyl-isothiocyanate
Authors	:	Schwartz, M.; Neiers, F.
Deposited on	:	2021-01-12
Resolution	:	2.46 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 following versions of software and data (see references (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.26
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 2.46 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	Similar resolution		
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
R_{free}	130704	1544 (2.48-2.44)		
Clashscore	141614	1613 (2.48-2.44)		
Ramachandran outliers	138981	1598 (2.48-2.44)		
Sidechain outliers	138945	1598 (2.48-2.44)		
RSRZ outliers	127900	1523 (2.48-2.44)		

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	А	222	5% 76%	14%	•	9%
1	В	222	3%	17%		• 5%
1	С	222	<mark>6%</mark> 75%	15%	•	9%
1	D	222	72%	21%		7%



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6681 atoms, of which 6 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.

Mol	Chain	Residues		Ate	oms			ZeroOcc	AltConf	Trace
1	Δ	201	Total	С	Ν	Ο	S	0	0	0
	A	201	1626	1057	272	290	$\overline{7}$	0	0	
1	р	210	Total	С	Ν	0	S	0	0	0
	D	210	1697	1101	282	306	8	0	0	U
1	C	202	Total	С	Ν	0	S	0	0	0
		205	1636	1061	273	294	8			
1	1 D	207	Total	С	Ν	0	S	0	0	0
	207	1674	1086	278	302	8	0	0	0	

• Molecule 1 is a protein called Glutathione S-transferase A1.

• Molecule 2 is N-prop-2-en-1-ylthioformamide (three-letter code: 9AI) (formula: C₄H₇NS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf		
0	В	1	Total	С	Η	Ν	\mathbf{S}	0	0
	D	1	12	4	6	1	1	0	0

• Molecule 3 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	10	Total O 10 10	0	0
3	В	9	Total O 9 9	0	0
3	С	11	Total O 11 11	0	0
3	D	6	Total O 6 6	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: Glutathione S-transferase A1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	100.11Å 94.65Å 104.51 Å	Deperitor
a, b, c, α , β , γ	90.00° 92.01° 90.00°	Depositor
$\mathbf{P}_{\text{acclution}}(\hat{\mathbf{A}})$	47.33 - 2.46	Depositor
Resolution (A)	47.33 - 2.46	EDS
% Data completeness	98.6 (47.33-2.46)	Depositor
(in resolution range)	99.0 (47.33-2.46)	EDS
R _{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.29 (at 2.45 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.17_3644	Depositor
D D	0.230 , 0.277	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.230 , 0.275	DCC
R_{free} test set	1765 reflections $(5.00%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	50.1	Xtriage
Anisotropy	0.563	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$< L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	0.001 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6681	wwPDB-VP
Average B, all atoms $(Å^2)$	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 63.42 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.6953e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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



¹Intensities estimated from amplitudes.

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: 9AI

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).

Mal	Chain	Bond	lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.50	0/1657	0.69	0/2226	
1	В	0.51	0/1731	0.65	0/2329	
1	С	0.59	0/1667	0.73	0/2241	
1	D	0.50	0/1708	0.75	0/2299	
All	All	0.52	0/6763	0.71	0/9095	

There are no bond length outliers.

There are no bond angle outliers.

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	А	1626	0	1698	35	0
1	В	1697	0	1766	34	0
1	С	1636	0	1696	27	0
1	D	1674	0	1738	34	0
2	В	6	6	6	0	0
3	А	10	0	0	0	0
3	В	9	0	0	0	0
3	С	11	0	0	0	0
3	D	6	0	0	2	0
All	All	6675	6	6904	119	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 9.

All (119) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom_1	Atom-2	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:A:117:LYS:HA	1:A:120:LYS:HE2	1.28	1.09	
1:D:102:LEU:HA	1:D:105:MET:HE3	1.40	1.02	
1:D:113:PRO:HB2	1:D:116:GLU:OE1	1.70	0.90	
1:B:183:ALA:O	1:B:187:ARG:HG3	1.73	0.87	
1:A:89:ARG:NE	1:B:89:ARG:HH12	1.81	0.78	
1:D:102:LEU:HA	1:D:105:MET:CE	2.16	0.73	
1:B:141:LYS:HG3	1:B:180:LEU:CD1	2.19	0.73	
1:D:116:GLU:HB3	1:D:120:LYS:NZ	2.04	0.72	
1:C:109:LEU:N	1:C:110:PRO:HD2	2.06	0.70	
1:A:117:LYS:CA	1:A:120:LYS:HE2	2.16	0.68	
1:D:109:LEU:HB3	1:D:110:PRO:HD3	1.76	0.67	
1:B:141:LYS:HG3	1:B:180:LEU:HD11	1.78	0.66	
1:A:175:ILE:HG12	1:A:182:LYS:HG2	1.79	0.65	
1:B:213:LEU:HD23	1:B:213:LEU:O	1.95	0.65	
1:A:109:LEU:CB	1:A:110:PRO:CD	2.75	0.65	
1:D:116:GLU:HB3	1:D:120:LYS:HZ3	1.63	0.63	
1:B:210:GLU:O	1:B:213:LEU:HB3	1.99	0.62	
1:C:111:VAL:HG23	1:C:111:VAL:O	1.99	0.61	
1:B:102:LEU:HD23	1:B:163:LEU:HD21	1.82	0.61	
1:B:82:TYR:CE1	1:B:89:ARG:HG3	2.36	0.60	
1:C:123:LEU:HD11	1:C:127:LYS:HE2	1.83	0.59	
1:D:182:LYS:O	1:D:186:THR:HG23	2.03	0.59	
1:D:82:TYR:CE1	1:D:89:ARG:HG3	2.38	0.58	
1:A:125:LYS:HG2	1:A:174:LEU:HD11	1.84	0.58	
1:D:102:LEU:HD23	1:D:163:LEU:HD21	1.84	0.57	
1:A:17:GLU:HG2	1:A:166:TYR:OH	2.04	0.57	
1:C:175:ILE:HG12	1:C:182:LYS:HG2	1.86	0.57	
1:B:141:LYS:HG3	1:B:180:LEU:HD12	1.85	0.57	
1:C:17:GLU:HG2	1:C:166:TYR:OH	2.06	0.55	
1:C:102:LEU:HD21	1:C:128:ILE:HG12	1.90	0.54	
1:A:39:GLU:O	1:A:43:LYS:HG3	2.07	0.54	
1:A:86:ILE:HD12	1:B:74:TYR:HE1	1.72	0.54	
1:A:109:LEU:HB3	1:A:110:PRO:HD3	1.90	0.54	
1:A:87:LYS:HD2	1:B:63:MET:HE1	1.89	0.54	
1:C:90:ALA:HA	3:D:305:HOH:O	2.08	0.54	
1:C:198:LEU:O	1:C:204:ARG:NH2	2.36	0.53	
1:A:128:ILE:O	1:A:133:PHE:HB2	2.08	0.53	

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		Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:D:102:LEU:HD21	1:D:128:ILE:HG12	1.89	0.53		
1:C:123:LEU:O	1:C:123:LEU:HG	2.07	0.52		
1:C:102:LEU:HD22	1:C:132:TYR:CD2	2.45	0.52		
1:D:90:ALA:HA	3:D:303:HOH:O	2.09	0.52		
1:D:66:VAL:O	1:D:67:GLN:HB2	2.10	0.51		
1:A:121:LEU:CD2	1:A:125:LYS:HD3	2.41	0.51		
1:B:72:LEU:HB3	1:B:155:ARG:NH2	2.25	0.51		
1:C:86:ILE:HG12	1:D:74:TYR:CD1	2.46	0.51		
1:D:17:GLU:HG2	1:D:166:TYR:OH	2.10	0.51		
1:D:175:ILE:HG12	1:D:182:LYS:HG2	1.92	0.51		
1:A:66:VAL:O	1:A:67:GLN:HB2	2.10	0.50		
1:B:200:PRO:HG3	1:D:204:ARG:CZ	2.42	0.50		
1:C:109:LEU:N	1:C:110:PRO:CD	2.74	0.50		
1:B:206:PRO:HA	1:D:200:PRO:HD2	1.93	0.50		
1:C:66:VAL:O	1:C:67:GLN:HB2	2.12	0.49		
1:D:164:LEU:HD22	1:D:175:ILE:HD12	1.94	0.49		
1:A:82:TYR:CE1	1:A:89:ARG:HG2	2.48	0.49		
1:C:128:ILE:O	1:C:133:PHE:HB2	2.12	0.49		
1:B:47:ASP:O	1:B:49:TYR:HD1	1.96	0.49		
1:C:127:LYS:O	1:C:131:ARG:HB3	2.13	0.48		
1:B:66:VAL:O	1:B:67:GLN:HB2	2.14	0.48		
1:A:84:LYS:HG2	1:A:88:GLU:OE1	2.13	0.48		
1:A:109:LEU:CB	1:A:110:PRO:HD3	2.42	0.48		
1:C:178:PHE:O	1:C:182:LYS:HG3	2.13	0.48		
1:C:208:MET:HG3	1:C:209:ASP:H	1.79	0.48		
1:A:95:TYR:HE1	1:B:51:MET:CE	2.27	0.47		
1:D:49:TYR:HB3	1:D:57:MET:HE2	1.96	0.47		
1:A:102:LEU:HD21	1:A:128:ILE:HG12	1.98	0.46		
1:B:109:LEU:HD21	1:B:121:LEU:HD13	1.97	0.46		
1:C:109:LEU:HD23	1:C:109:LEU:HA	1.61	0.46		
1:A:121:LEU:C	1:A:121:LEU:HD23	2.36	0.46		
1:A:86:ILE:HD12	1:A:87:LYS:HG2	1.97	0.46		
1:A:120:LYS:HE3	1:A:120:LYS:HB2	1.47	0.46		
1:B:145:GLN:CD	1:B:151:ASN:HB2	2.36	0.45		
1:D:198:LEU:O	1:D:204:ARG:NH2	2.40	0.45		
1:D:116:GLU:HB3	1:D:120:LYS:HZ2	1.80	0.45		
1:B:63:MET:HE1	1:B:74:TYR:CE1	2.52	0.45		
1:D:112:CYS:SG	1:D:120:LYS:HD3	2.57	0.45		
1:A:9:TYR:HE1	1:A:56:PRO:HD3	1.82	0.44		
1:A:87:LYS:HD2	1:B:63:MET:CE	2.47	0.44		
1:B:182:LYS:O	1:B:186:THR:HG23	2.17	0.44		

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	te as page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:9:TYR:HB2	1:A:16:MET:CE	2.47	0.44
1:B:84:LYS:HG3	1:B:88:GLU:OE1	2.16	0.44
1:B:120:LYS:HA	1:B:120:LYS:HD3	1.51	0.44
1:B:4:LYS:HB2	1:B:4:LYS:HE2	1.85	0.44
1:A:95:TYR:HE1	1:B:51:MET:HE1	1.82	0.43
1:B:125:LYS:HG2	1:B:174:LEU:HD11	2.00	0.43
1:A:86:ILE:HD12	1:B:74:TYR:CE1	2.53	0.43
1:C:82:TYR:CD1	1:C:89:ARG:HG2	2.54	0.43
1:D:112:CYS:HB2	1:D:120:LYS:HE2	2.01	0.43
1:C:28:VAL:HG21	1:C:79:TYR:CZ	2.53	0.43
1:B:102:LEU:HD21	1:B:128:ILE:HG12	2.01	0.43
1:C:208:MET:HG3	1:C:209:ASP:N	2.33	0.43
1:D:161:VAL:HG21	1:D:188:ILE:HB	2.01	0.43
1:A:28:VAL:HG21	1:A:79:TYR:CZ	2.53	0.43
1:C:96:ILE:HA	1:C:99:ILE:HD12	2.01	0.42
1:B:17:GLU:HG2	1:B:166:TYR:OH	2.19	0.42
1:D:72:LEU:HB3	1:D:155:ARG:NH2	2.35	0.42
1:D:126:GLU:HG2	1:D:130:ASN:OD1	2.19	0.42
1:C:35:ILE:HD11	1:C:55:VAL:HG11	2.01	0.42
1:D:28:VAL:HG21	1:D:79:TYR:CZ	2.54	0.42
1:B:145:GLN:HG2	1:B:151:ASN:CG	2.40	0.42
1:D:148:LEU:HD11	1:D:160:LEU:HD23	2.01	0.42
1:C:49:TYR:CE1	1:C:64:LYS:HE3	2.54	0.42
1:C:174:LEU:HA	1:C:174:LEU:HD23	1.87	0.42
1:A:109:LEU:N	1:A:110:PRO:HD2	2.34	0.41
1:B:47:ASP:HB3	1:B:49:TYR:CD1	2.55	0.41
1:B:47:ASP:HB3	1:B:49:TYR:CE1	2.55	0.41
1:D:28:VAL:HG21	1:D:79:TYR:CE2	2.55	0.41
1:A:86:ILE:CD1	1:A:87:LYS:HG2	2.50	0.41
1:D:174:LEU:HA	1:D:174:LEU:HD23	1.78	0.41
1:A:121:LEU:HD23	1:A:125:LYS:HD3	2.03	0.41
1:C:82:TYR:O	1:C:89:ARG:HG3	2.21	0.41
1:D:4:LYS:HE3	1:D:4:LYS:HB3	1.90	0.41
1:A:9:TYR:CE1	1:A:56:PRO:HD3	2.55	0.41
1:A:174:LEU:HA	1:A:174:LEU:HD23	1.85	0.41
1:C:127:LYS:NZ	1:C:131:ARG:NH1	2.69	0.41
1:D:127:LYS:O	1:D:131:ARG:HB3	2.21	0.41
1:A:94:MET:SD	1:B:66:VAL:HG22	2.61	0.41
1:D:148:LEU:HD11	1:D:160:LEU:CD2	2.50	0.40
1:D:171:ASP:HB3	1:D:174:LEU:CD1	2.51	0.40
1:A:28:VAL:HG21	1:A:79:TYR:CE2	2.56	0.40

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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	Perce	entiles
1	А	197/222~(89%)	192~(98%)	5(2%)	0	100	100
1	В	208/222~(94%)	201~(97%)	7 (3%)	0	100	100
1	С	199/222~(90%)	190 (96%)	9~(4%)	0	100	100
1	D	205/222 (92%)	199~(97%)	5(2%)	1 (0%)	29	34
All	All	809/888~(91%)	782(97%)	26(3%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	114	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	176/196~(90%)	171 (97%)	5(3%)	43 56
1	В	186/196~(95%)	177 (95%)	9~(5%)	25 33
1	С	177/196~(90%)	171 (97%)	6 (3%)	37 48
1	D	183/196~(93%)	178 (97%)	5(3%)	44 57
All	All	722/784~(92%)	697~(96%)	25~(4%)	36 47



Mol	Chain	Res	Type
1	А	33	LYS
1	А	36	LYS
1	А	43	LYS
1	А	82	TYR
1	А	120	LYS
1	В	4	LYS
1	В	10	PHE
1	В	43	LYS
1	В	82	TYR
1	В	84	LYS
1	В	120	LYS
1	В	142	SER
1	В	208	MET
1	В	211	LYS
1	С	6	LYS
1	С	82	TYR
1	С	109	LEU
1	С	112	CYS
1	С	123	LEU
1	С	126	GLU
1	D	6	LYS
1	D	43	LYS
1	D	82	TYR
1	D	173	SER
1	D	196	LYS

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

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)

1 ligand is 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).

Mal	Type	Chain	Dog	Link	B	ond leng	gths	В	Sond ang	gles
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	9AI	В	401	1	5,5,5	1.02	1 (20%)	$2,\!4,\!4$	0.51	0

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	9AI	В	401	1	-	1/1/3/3	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	401	9AI	C1-N1	2.12	1.38	1.31

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	В	401	9AI	C4-C5-C6-N1

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 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.



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ $>$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	201/222 (90%)	0.47	11 (5%) 25 22	35, 52, 72, 94	0
1	В	210/222 (94%)	0.30	7 (3%) 46 43	39, 53, 78, 101	0
1	С	203/222 (91%)	0.57	13 (6%) 19 16	31, 46, 78, 94	0
1	D	207/222 (93%)	0.45	10 (4%) 30 28	33, 51, 85, 96	0
All	All	821/888 ($92%$)	0.45	41 (4%) 28 26	31, 51, 80, 101	0

All (41) RSRZ outliers are listed below:

Mol	Chain	\mathbf{Res}	Type	RSRZ
1	С	110	PRO	6.7
1	D	10	PHE	4.6
1	А	117	LYS	4.3
1	D	110	PRO	4.2
1	С	121	LEU	4.1
1	D	38	ALA	4.0
1	С	2	ALA	3.8
1	В	211	LYS	3.8
1	А	109	LEU	3.8
1	С	108	LEU	3.6
1	В	212	SER	3.5
1	D	41	LEU	3.4
1	А	110	PRO	3.4
1	С	111	VAL	3.3
1	А	10	PHE	3.3
1	С	107	LEU	3.3
1	А	118	ASP	3.3
1	А	41	LEU	3.2
1	В	213	LEU	3.1
1	А	123	LEU	3.0
1	В	37	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	С	170	LEU	2.9
1	D	114	PRO	2.8
1	D	37	SER	2.8
1	С	208	MET	2.8
1	А	120	LYS	2.7
1	С	3	GLU	2.6
1	D	112	CYS	2.6
1	В	71	ILE	2.5
1	D	35	ILE	2.4
1	В	43	LYS	2.4
1	С	123	LEU	2.4
1	А	3	GLU	2.4
1	D	113	PRO	2.2
1	А	42	ASP	2.2
1	А	174	LEU	2.2
1	В	44	LEU	2.2
1	С	10	PHE	2.1
1	D	53	GLN	2.1
1	С	127	LYS	2.0
1	С	103	GLY	2.0

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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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
2	9AI	В	401	6/6	0.74	0.18	61,73,88,88	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.

