Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 11:35 am GMT

PDB ID	:	2XO8
Title	:	Crystal Structure of Myosin-2 in Complex with Tribromodichloropseudilin
Authors	:	Preller, M.; Chinthalapudi, K.; Martin, R.; Knoelker, H.J.; Manstein, D.J.
Deposited on	:	2010-08-10
Resolution	:	2.40 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:

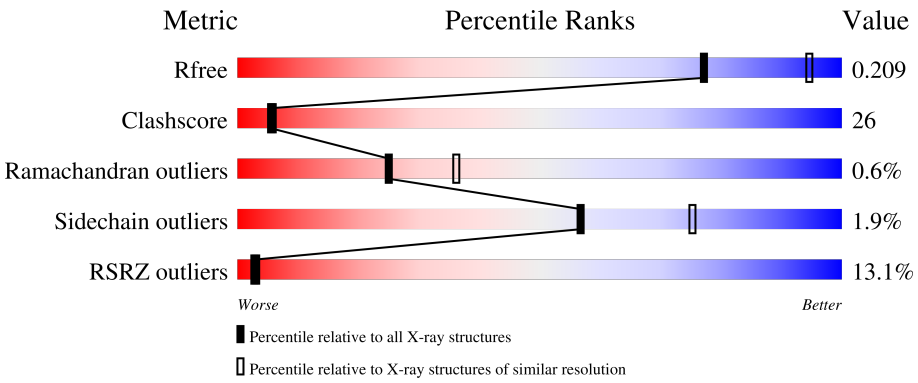
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	776	13% 65% 33% •

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	H70	A	1778	-	-	X	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 6720 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.

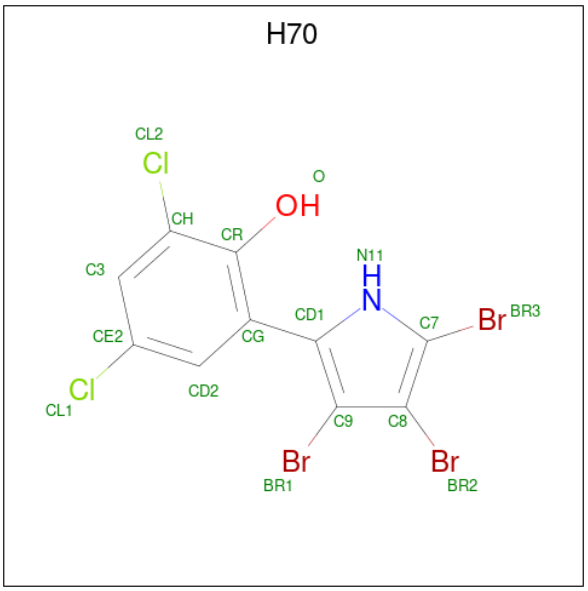
- Molecule 1 is a protein called MYOSIN-2 HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	776	6236	3961	1071	1187	17	36	0	0

There are 19 discrepancies between the modelled and reference sequences:

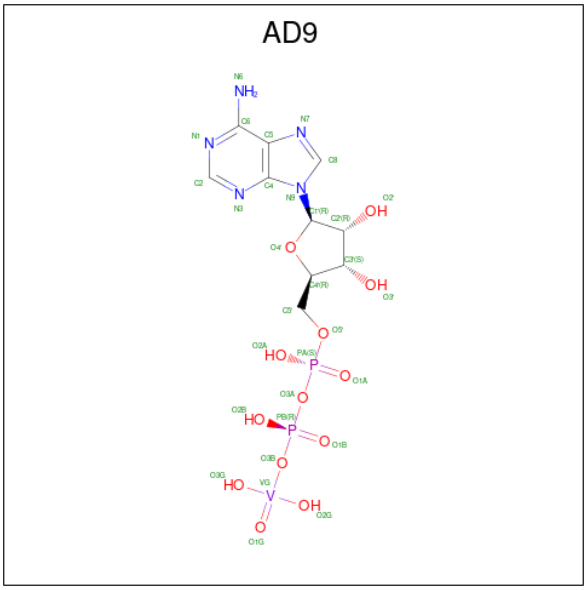
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ASP	-	expression tag	UNP P08799
A	762	LEU	-	expression tag	UNP P08799
A	763	GLU	-	expression tag	UNP P08799
A	764	SER	-	expression tag	UNP P08799
A	765	ASN	-	expression tag	UNP P08799
A	766	GLU	-	expression tag	UNP P08799
A	767	PRO	-	expression tag	UNP P08799
A	768	PRO	-	expression tag	UNP P08799
A	769	MET	-	expression tag	UNP P08799
A	770	ASP	-	expression tag	UNP P08799
A	771	PHE	-	expression tag	UNP P08799
A	772	ASP	-	expression tag	UNP P08799
A	773	ASP	-	expression tag	UNP P08799
A	774	ASP	-	expression tag	UNP P08799
A	775	ILE	-	expression tag	UNP P08799
A	776	PRO	-	expression tag	UNP P08799
A	777	PHE	-	expression tag	UNP P08799
A	131	ILE	ARG	conflict	UNP P08799
A	435	ILE	LYS	conflict	UNP P08799

- Molecule 2 is 2,4-DICHLORO-6-(3,4,5-TRIBROMO-1H-PYRROL-2-YL)PHENOL (three-letter code: H70) (formula: $C_{10}H_4Br_3Cl_2NO$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	Br	C	Cl	N	O		
2	A	1	17	3	10	2	1	1	0	0

- Molecule 3 is ADP METAVANADATE (three-letter code: AD9) (formula: $C_{10}H_{16}N_5O_{13}P_2V$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	V		
3	A	1	31	10	5	13	2	1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	1	1	1	0	0

- Molecule 5 is water.

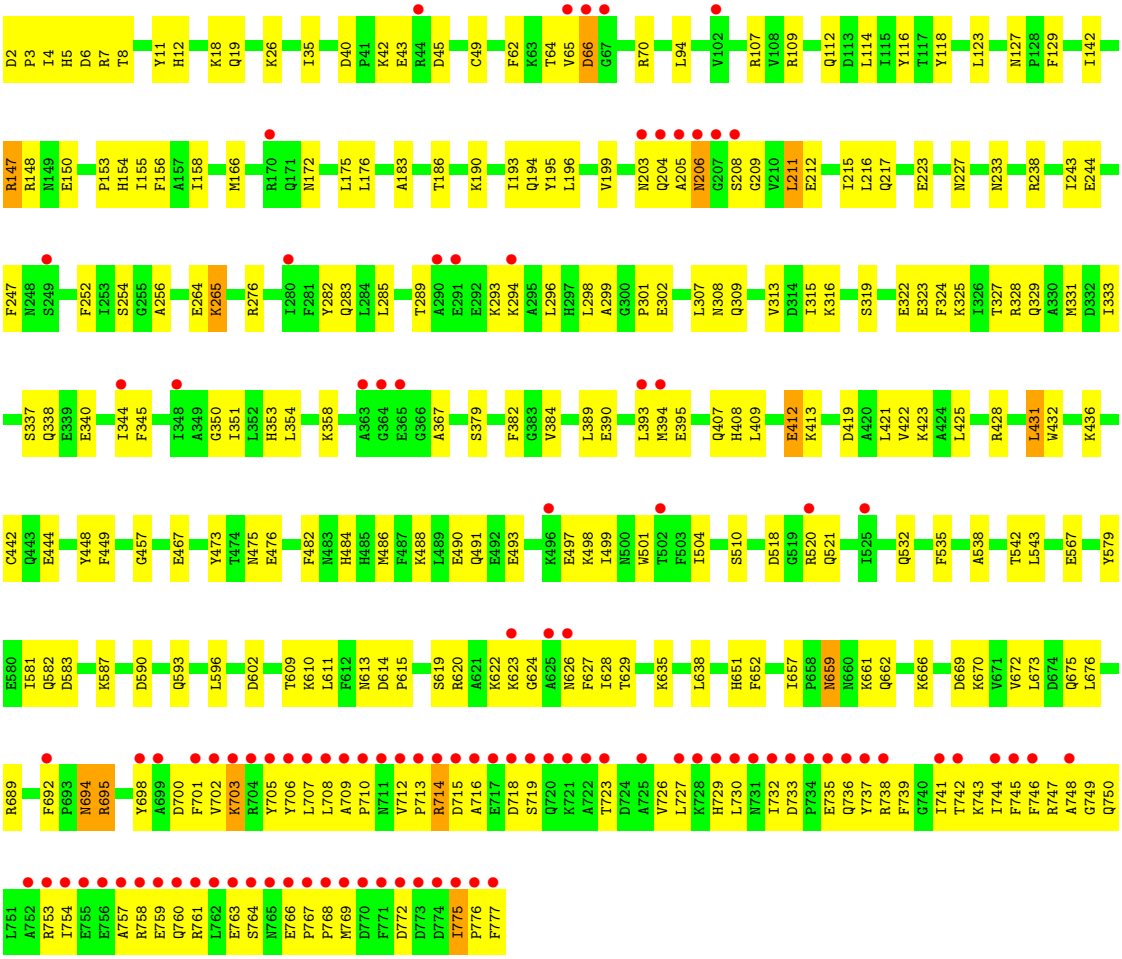
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	435	435	435	0	0

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: MYOSIN-2 HEAVY CHAIN

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	88.34Å 146.38Å 152.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.70 – 2.40 19.69 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.70-2.40) 99.9 (19.69-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.07 (at 2.41Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.202 , 0.254 0.203 , 0.209	Depositor DCC
R_{free} test set	1949 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	39.9	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 47.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.029 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.036 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6720	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: H70, MG, AD9

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	0.48	4/6361 (0.1%)	0.63	10/8587 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	265	LYS	CB-CG	-9.72	1.26	1.52
1	A	265	LYS	CG-CD	-7.69	1.26	1.52
1	A	265	LYS	CD-CE	-7.32	1.32	1.51
1	A	265	LYS	CE-NZ	-5.02	1.36	1.49

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	412	GLU	CB-CA-C	-7.49	95.42	110.40
1	A	206	ASN	N-CA-C	7.42	131.04	111.00
1	A	769	MET	CB-CA-C	6.92	124.25	110.40
1	A	703	LYS	CB-CA-C	-6.62	97.15	110.40
1	A	66	ASP	CB-CA-C	-6.35	97.69	110.40
1	A	703	LYS	N-CA-C	5.98	127.16	111.00
1	A	412	GLU	N-CA-C	5.44	125.69	111.00
1	A	337	SER	CB-CA-C	-5.23	100.16	110.10
1	A	431	LEU	CA-CB-CG	-5.12	103.52	115.30
1	A	233	ASN	CB-CA-C	5.07	120.54	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	6236	0	6168	315	1
2	A	17	0	4	17	0
3	A	31	0	13	1	0
4	A	1	0	0	0	0
5	A	435	0	0	80	0
All	All	6720	0	6185	320	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 26.

All (320) 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:761:ARG:HD2	1:A:764:SER:CB	1.23	1.61
1:A:761:ARG:CD	1:A:764:SER:HB3	1.33	1.57
1:A:743:LYS:HE3	5:A:2428:HOH:O	1.25	1.34
1:A:761:ARG:CD	1:A:764:SER:CB	1.94	1.28
1:A:700:ASP:HB2	5:A:2414:HOH:O	1.12	1.26
1:A:761:ARG:NH1	1:A:764:SER:HB2	1.54	1.18
1:A:294:LYS:HA	5:A:2186:HOH:O	1.46	1.12
1:A:265:LYS:NZ	2:A:1778:H70:H11	1.47	1.11
1:A:42:LYS:HA	5:A:2038:HOH:O	1.52	1.09
2:A:1778:H70:CL1	5:A:2268:HOH:O	2.10	1.04
1:A:265:LYS:HE3	2:A:1778:H70:HD2	1.06	1.03
1:A:265:LYS:CE	2:A:1778:H70:HD2	1.87	1.02
1:A:761:ARG:CD	1:A:764:SER:HB2	1.82	1.01
1:A:761:ARG:HH11	1:A:764:SER:HB2	1.14	1.01
1:A:772:ASP:HB3	1:A:776:PRO:HG3	1.41	1.01
1:A:761:ARG:CZ	1:A:764:SER:HB2	1.91	1.00
1:A:659:ASN:HD22	1:A:661:LYS:H	1.11	0.99
1:A:18:LYS:H	1:A:112:GLN:HE22	1.10	0.97
1:A:154:HIS:CD2	1:A:156:PHE:H	1.81	0.97
1:A:265:LYS:NZ	2:A:1778:H70:N11	2.13	0.97
1:A:293:LYS:HD2	5:A:2185:HOH:O	1.65	0.96
1:A:615:PRO:O	1:A:619:SER:HB2	1.66	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:ASN:HD21	1:A:749:GLY:HA2	1.28	0.95
1:A:265:LYS:HE3	2:A:1778:H70:CD2	1.96	0.95
1:A:118:TYR:CG	1:A:148:ARG:NH2	2.35	0.94
1:A:107:ARG:HD3	5:A:2091:HOH:O	1.65	0.94
1:A:491:GLN:HE21	1:A:501:TRP:HE1	1.06	0.92
1:A:491:GLN:HE22	1:A:504:ILE:H	1.03	0.91
1:A:265:LYS:HZ2	2:A:1778:H70:H11	1.10	0.91
1:A:118:TYR:HB3	1:A:148:ARG:NH2	1.88	0.88
1:A:64:THR:O	1:A:66:ASP:O	1.92	0.88
1:A:431:LEU:CD1	5:A:2271:HOH:O	2.20	0.88
1:A:718:ASP:C	5:A:2423:HOH:O	2.11	0.88
1:A:204:GLN:HG2	5:A:2149:HOH:O	1.72	0.87
1:A:118:TYR:CD1	1:A:148:ARG:NH2	2.42	0.86
1:A:154:HIS:HD2	1:A:156:PHE:H	0.89	0.86
1:A:206:ASN:OD1	1:A:206:ASN:O	1.92	0.86
1:A:520:ARG:HH11	1:A:521:GLN:HE21	1.22	0.86
2:A:1778:H70:BR3	5:A:2171:HOH:O	2.47	0.85
1:A:657:ILE:H	1:A:675:GLN:HE22	1.18	0.85
1:A:761:ARG:NE	1:A:764:SER:CB	2.40	0.85
1:A:154:HIS:HD2	1:A:156:PHE:N	1.74	0.84
1:A:118:TYR:HB3	1:A:148:ARG:HH22	1.43	0.83
1:A:431:LEU:HG	5:A:2271:HOH:O	1.80	0.82
1:A:431:LEU:HD11	5:A:2271:HOH:O	1.79	0.82
1:A:147:ARG:HD3	1:A:147:ARG:H	1.44	0.81
1:A:431:LEU:HD22	2:A:1778:H70:BR2	2.36	0.81
1:A:294:LYS:HD3	5:A:2186:HOH:O	1.79	0.80
1:A:703:LYS:NZ	5:A:2416:HOH:O	2.14	0.80
1:A:294:LYS:CD	5:A:2186:HOH:O	2.31	0.79
1:A:747:ARG:HD3	5:A:2413:HOH:O	1.82	0.79
1:A:431:LEU:CG	5:A:2271:HOH:O	2.31	0.79
1:A:609:THR:HG23	1:A:613:ASN:HD22	1.48	0.79
1:A:609:THR:HG23	1:A:613:ASN:ND2	1.98	0.79
1:A:761:ARG:NE	1:A:764:SER:HB2	1.98	0.79
1:A:764:SER:HA	1:A:768:PRO:HG2	1.63	0.78
1:A:741:ILE:HG22	1:A:742:THR:HG23	1.64	0.78
1:A:692:PHE:HB3	1:A:745:PHE:HB3	1.66	0.77
1:A:520:ARG:NH1	1:A:521:GLN:HE21	1.81	0.77
1:A:118:TYR:CB	1:A:148:ARG:NH2	2.47	0.77
1:A:761:ARG:CZ	1:A:764:SER:CB	2.65	0.75
1:A:709:ALA:HB1	1:A:710:PRO:HD2	1.69	0.75
1:A:750:GLN:HE22	1:A:753:ARG:HE	1.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:LYS:HD2	5:A:2022:HOH:O	1.88	0.74
1:A:42:LYS:O	5:A:2038:HOH:O	2.04	0.74
1:A:294:LYS:CA	5:A:2186:HOH:O	2.15	0.74
1:A:206:ASN:N	5:A:2153:HOH:O	2.21	0.74
1:A:276:ARG:NH1	5:A:2180:HOH:O	2.22	0.73
1:A:442:CYS:HB3	5:A:2274:HOH:O	1.89	0.73
1:A:294:LYS:CB	5:A:2186:HOH:O	2.34	0.73
1:A:491:GLN:NE2	1:A:504:ILE:H	1.81	0.73
1:A:5:HIS:HD2	5:A:2001:HOH:O	1.71	0.73
1:A:761:ARG:HG3	1:A:763:GLU:O	1.88	0.73
1:A:733:ASP:HB3	1:A:736:GLN:HB2	1.69	0.72
1:A:172:ASN:ND2	1:A:449:PHE:H	1.88	0.71
1:A:694:ASN:ND2	1:A:749:GLY:HA2	2.05	0.71
1:A:746:PHE:C	5:A:2429:HOH:O	2.28	0.71
1:A:491:GLN:HE22	1:A:504:ILE:N	1.85	0.71
1:A:45:ASP:HB3	1:A:673:LEU:HD12	1.73	0.70
1:A:42:LYS:CA	5:A:2038:HOH:O	2.22	0.70
1:A:719:SER:N	5:A:2423:HOH:O	2.21	0.70
1:A:431:LEU:HD21	5:A:2381:HOH:O	1.92	0.69
1:A:421:LEU:O	1:A:425:LEU:HG	1.92	0.69
1:A:610:LYS:HE3	1:A:614:ASP:OD2	1.92	0.69
1:A:659:ASN:ND2	1:A:661:LYS:H	1.87	0.69
1:A:761:ARG:CD	1:A:763:GLU:O	2.41	0.69
1:A:623:LYS:HE2	1:A:628:ILE:HA	1.75	0.68
1:A:147:ARG:HE	1:A:150:GLU:HB2	1.56	0.68
1:A:5:HIS:CD2	5:A:2001:HOH:O	2.44	0.68
1:A:65:VAL:O	5:A:2060:HOH:O	2.11	0.67
1:A:518:ASP:HB2	1:A:635:LYS:HE3	1.77	0.67
1:A:709:ALA:HA	1:A:729:HIS:CD2	2.30	0.66
1:A:205:ALA:HB1	5:A:2150:HOH:O	1.95	0.66
1:A:316:LYS:HG3	5:A:2197:HOH:O	1.96	0.66
1:A:610:LYS:HD2	1:A:614:ASP:HB2	1.77	0.65
1:A:285:LEU:O	5:A:2181:HOH:O	2.14	0.65
1:A:293:LYS:CD	5:A:2185:HOH:O	2.32	0.65
1:A:206:ASN:CA	5:A:2153:HOH:O	2.44	0.65
1:A:750:GLN:NE2	1:A:753:ARG:HE	1.95	0.65
1:A:761:ARG:NH1	1:A:764:SER:CB	2.47	0.65
1:A:294:LYS:HE2	5:A:2186:HOH:O	1.98	0.64
1:A:623:LYS:HZ3	1:A:629:THR:H	1.45	0.64
1:A:325:LYS:O	1:A:329:GLN:HG3	1.98	0.64
1:A:758:ARG:HA	1:A:761:ARG:HH21	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:LYS:CD	5:A:2022:HOH:O	2.44	0.63
1:A:714:ARG:NH2	5:A:2418:HOH:O	2.29	0.63
2:A:1778:H70:C3	5:A:2268:HOH:O	2.47	0.63
1:A:623:LYS:HD3	1:A:628:ILE:HG13	1.80	0.63
1:A:748:ALA:HB3	1:A:753:ARG:NH2	2.13	0.62
2:A:1778:H70:H3	5:A:2268:HOH:O	1.99	0.62
1:A:285:LEU:HD11	1:A:307:LEU:CD1	2.30	0.62
1:A:718:ASP:CG	5:A:2423:HOH:O	2.38	0.62
1:A:294:LYS:CE	5:A:2186:HOH:O	2.48	0.61
1:A:276:ARG:NH2	1:A:282:TYR:CD2	2.67	0.61
1:A:193:ILE:HD11	1:A:243:ILE:HD13	1.81	0.61
1:A:285:LEU:CD1	1:A:307:LEU:CD1	2.79	0.61
1:A:358:LYS:HE3	5:A:2220:HOH:O	2.01	0.61
1:A:730:LEU:H	1:A:758:ARG:HH22	1.48	0.61
1:A:761:ARG:HD3	1:A:764:SER:CB	2.20	0.61
1:A:324:PHE:O	1:A:328:ARG:HG3	2.02	0.60
1:A:195:TYR:CZ	1:A:199:VAL:HG21	2.37	0.59
1:A:775:ILE:N	1:A:776:PRO:CD	2.65	0.59
1:A:431:LEU:HD13	2:A:1778:H70:BR2	2.57	0.59
1:A:761:ARG:CG	1:A:763:GLU:O	2.51	0.59
1:A:18:LYS:H	1:A:112:GLN:NE2	1.91	0.59
1:A:293:LYS:NZ	5:A:2185:HOH:O	2.26	0.59
1:A:203:ASN:HB2	5:A:2153:HOH:O	2.01	0.58
1:A:254:SER:HB2	1:A:444:GLU:HG2	1.84	0.58
1:A:289:THR:HG21	5:A:2183:HOH:O	2.04	0.58
1:A:520:ARG:NH1	1:A:521:GLN:NE2	2.50	0.58
1:A:45:ASP:CB	1:A:673:LEU:HD12	2.34	0.58
1:A:763:GLU:HA	1:A:767:PRO:HG2	1.84	0.58
1:A:657:ILE:N	1:A:675:GLN:HE22	1.96	0.57
1:A:738:ARG:O	1:A:744:ILE:HD12	2.04	0.57
1:A:276:ARG:HH11	1:A:315:ILE:HD11	1.69	0.57
1:A:623:LYS:NZ	1:A:629:THR:H	2.02	0.57
1:A:532:GLN:NE2	1:A:542:THR:C	2.58	0.57
1:A:209:GLY:O	1:A:212:GLU:OE1	2.23	0.57
1:A:428:ARG:NH2	2:A:1778:H70:CL2	2.67	0.57
1:A:730:LEU:HB3	1:A:758:ARG:HH12	1.70	0.57
1:A:175:LEU:HD13	1:A:651:HIS:HB2	1.87	0.56
1:A:276:ARG:NH1	1:A:315:ILE:HD11	2.19	0.56
1:A:293:LYS:CE	5:A:2185:HOH:O	2.53	0.56
1:A:532:GLN:HE21	1:A:543:LEU:N	2.03	0.56
1:A:620:ARG:HG2	1:A:627:PHE:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:ASP:OD1	2:A:1778:H70:CL1	2.60	0.56
1:A:767:PRO:HB2	1:A:768:PRO:HD3	1.86	0.56
1:A:289:THR:CG2	5:A:2183:HOH:O	2.53	0.56
1:A:730:LEU:H	1:A:758:ARG:NH2	2.03	0.56
1:A:389:LEU:O	1:A:393:LEU:HG	2.05	0.56
1:A:491:GLN:NE2	1:A:501:TRP:HE1	1.89	0.56
1:A:735:GLU:HB2	5:A:2425:HOH:O	2.05	0.56
1:A:172:ASN:HD21	1:A:448:TYR:HA	1.70	0.55
1:A:670:LYS:HB2	5:A:2017:HOH:O	2.07	0.55
1:A:497:GLU:HG3	1:A:745:PHE:HZ	1.71	0.55
1:A:622:LYS:HE3	1:A:624:GLY:O	2.06	0.54
1:A:285:LEU:HD22	1:A:299:ALA:O	2.07	0.54
1:A:26:LYS:HE3	5:A:2022:HOH:O	2.08	0.54
1:A:204:GLN:NE2	5:A:2149:HOH:O	2.32	0.54
1:A:532:GLN:HG3	1:A:538:ALA:HB1	1.90	0.54
1:A:741:ILE:HG22	1:A:742:THR:CG2	2.34	0.54
1:A:94:LEU:O	1:A:689:ARG:NH1	2.41	0.54
1:A:265:LYS:HB3	1:A:423:LYS:HB3	1.89	0.54
1:A:694:ASN:HD22	1:A:746:PHE:HB2	1.71	0.54
1:A:393:LEU:HD23	1:A:596:LEU:HD21	1.89	0.54
1:A:707:LEU:HG	1:A:712:VAL:H	1.72	0.53
1:A:209:GLY:HA3	5:A:2145:HOH:O	2.07	0.53
1:A:395:GLU:HA	1:A:407:GLN:O	2.09	0.53
1:A:775:ILE:H	1:A:776:PRO:HD3	1.71	0.53
1:A:623:LYS:N	1:A:626:ASN:O	2.42	0.52
1:A:476:GLU:OE2	1:A:510:SER:HB2	2.09	0.52
1:A:484:HIS:HD2	1:A:488:LYS:HD3	1.74	0.52
1:A:761:ARG:HD3	1:A:764:SER:HB2	1.81	0.52
1:A:510:SER:HA	5:A:2309:HOH:O	2.09	0.52
1:A:761:ARG:HD2	1:A:763:GLU:O	2.10	0.52
1:A:319:SER:O	1:A:323:GLU:HG2	2.10	0.52
1:A:763:GLU:HG3	1:A:767:PRO:HB2	1.92	0.52
1:A:698:TYR:CD2	1:A:723:THR:HG21	2.45	0.52
1:A:766:GLU:N	1:A:767:PRO:CD	2.72	0.52
1:A:532:GLN:NE2	1:A:542:THR:OG1	2.43	0.51
1:A:265:LYS:CE	2:A:1778:H70:H11	2.19	0.51
1:A:432:TRP:CZ2	1:A:436:LYS:HE3	2.45	0.51
1:A:247:PHE:HA	1:A:252:PHE:O	2.10	0.51
1:A:497:GLU:HG3	1:A:745:PHE:CZ	2.46	0.51
1:A:203:ASN:C	5:A:2153:HOH:O	2.48	0.51
1:A:535:PHE:HD2	1:A:538:ALA:HB2	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:GLU:HG3	5:A:2425:HOH:O	2.11	0.51
1:A:746:PHE:HB3	1:A:750:GLN:HB2	1.93	0.51
1:A:409:LEU:HB3	1:A:413:LYS:HB3	1.93	0.50
1:A:338:GLN:HG3	5:A:2213:HOH:O	2.11	0.50
1:A:436:LYS:HG3	5:A:2272:HOH:O	2.11	0.50
1:A:710:PRO:O	1:A:712:VAL:HG12	2.12	0.50
1:A:747:ARG:C	5:A:2429:HOH:O	2.50	0.50
1:A:739:PHE:CD1	1:A:744:ILE:HD13	2.46	0.50
1:A:467:GLU:OE2	1:A:587:LYS:HE2	2.12	0.50
1:A:2:ASP:OD1	1:A:3:PRO:HD2	2.11	0.50
1:A:223:GLU:O	1:A:227:ASN:HB2	2.12	0.50
1:A:692:PHE:CB	1:A:745:PHE:HB3	2.38	0.49
1:A:705:TYR:HB3	1:A:726:VAL:HG11	1.94	0.49
1:A:723:THR:O	1:A:727:LEU:HD13	2.11	0.49
1:A:109:ARG:HB3	1:A:114:LEU:HB2	1.93	0.49
1:A:673:LEU:HD23	1:A:676:LEU:HD12	1.94	0.49
1:A:4:ILE:HA	1:A:11:TYR:CD2	2.48	0.49
1:A:147:ARG:HD3	1:A:147:ARG:N	2.19	0.49
1:A:166:MET:SD	1:A:247:PHE:CD2	3.06	0.49
1:A:205:ALA:CA	5:A:2150:HOH:O	2.61	0.49
1:A:672:VAL:O	1:A:676:LEU:HG	2.12	0.49
1:A:532:GLN:NE2	1:A:543:LEU:N	2.61	0.49
1:A:186:THR:O	1:A:190:LYS:HG3	2.13	0.49
1:A:26:LYS:CE	5:A:2022:HOH:O	2.61	0.49
1:A:193:ILE:HD11	1:A:243:ILE:CD1	2.43	0.49
1:A:238:ARG:HD3	1:A:264:GLU:OE1	2.13	0.49
1:A:367:ALA:O	1:A:408:HIS:HE1	1.95	0.48
1:A:457:GLY:N	3:A:1779:AD9:O2G	2.43	0.48
1:A:718:ASP:CB	5:A:2423:HOH:O	2.60	0.48
1:A:147:ARG:H	1:A:147:ARG:CD	2.18	0.48
1:A:764:SER:CA	1:A:768:PRO:HG2	2.40	0.48
1:A:211:LEU:O	1:A:215:ILE:HG13	2.12	0.48
1:A:694:ASN:HD21	1:A:749:GLY:CA	2.14	0.48
1:A:7:ARG:NH1	1:A:19:GLN:OE1	2.46	0.48
1:A:350:GLY:HA3	1:A:382:PHE:CZ	2.49	0.48
1:A:40:ASP:OD1	1:A:42:LYS:HB2	2.14	0.48
1:A:354:LEU:HD11	1:A:425:LEU:HD11	1.95	0.48
1:A:757:ALA:O	1:A:761:ARG:NE	2.47	0.48
1:A:709:ALA:HB2	1:A:726:VAL:HA	1.96	0.48
1:A:206:ASN:O	1:A:206:ASN:CG	2.53	0.47
1:A:351:ILE:HG23	1:A:422:VAL:HG13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:ARG:O	1:A:695:ARG:HG2	2.15	0.47
1:A:350:GLY:O	1:A:354:LEU:HG	2.13	0.47
1:A:567:GLU:HA	1:A:579:TYR:O	2.15	0.47
1:A:282:TYR:CE1	1:A:307:LEU:HD22	2.50	0.47
1:A:692:PHE:CZ	1:A:747:ARG:NH2	2.83	0.47
1:A:129:PHE:CE2	1:A:662:GLN:HA	2.50	0.46
1:A:733:ASP:OD1	1:A:735:GLU:HG2	2.16	0.46
1:A:276:ARG:NH2	1:A:282:TYR:CG	2.83	0.46
1:A:217:GLN:HG3	1:A:333:ILE:HG21	1.97	0.46
1:A:296:LEU:HB2	1:A:298:LEU:HG	1.98	0.46
1:A:302:GLU:H	1:A:302:GLU:CD	2.18	0.46
1:A:749:GLY:N	5:A:2429:HOH:O	2.47	0.46
1:A:775:ILE:N	1:A:776:PRO:HD3	2.29	0.46
1:A:244:GLU:O	1:A:256:ALA:HA	2.16	0.46
1:A:204:GLN:HG2	5:A:2147:HOH:O	1.77	0.46
1:A:390:GLU:HG3	1:A:394:MET:CE	2.45	0.46
1:A:457:GLY:HA2	1:A:475:ASN:HD21	1.80	0.46
1:A:709:ALA:CB	1:A:726:VAL:HA	2.46	0.46
1:A:296:LEU:O	1:A:353:HIS:HE1	1.99	0.46
1:A:490:GLU:O	1:A:493:GLU:HB3	2.15	0.46
1:A:535:PHE:CD2	1:A:538:ALA:HB2	2.51	0.46
1:A:777:PHE:CD1	1:A:777:PHE:OXT	2.69	0.46
1:A:26:LYS:NZ	5:A:2024:HOH:O	2.47	0.46
1:A:498:LYS:HD3	1:A:741:ILE:HD11	1.98	0.46
1:A:6:ASP:OD1	1:A:8:THR:HB	2.14	0.46
1:A:254:SER:HB2	1:A:444:GLU:CG	2.46	0.46
1:A:328:ARG:NH2	5:A:2208:HOH:O	2.49	0.46
1:A:331:MET:HE3	1:A:345:PHE:HZ	1.81	0.45
1:A:340:GLU:O	1:A:344:ILE:HG13	2.16	0.45
1:A:205:ALA:CB	5:A:2150:HOH:O	2.57	0.45
1:A:766:GLU:H	1:A:767:PRO:CD	2.28	0.45
1:A:301:PRO:HB2	1:A:313:VAL:HG11	1.98	0.45
1:A:614:ASP:OD1	1:A:614:ASP:C	2.55	0.45
1:A:666:LYS:NZ	5:A:2400:HOH:O	2.49	0.45
1:A:6:ASP:C	1:A:8:THR:H	2.19	0.45
1:A:484:HIS:CD2	1:A:488:LYS:HD3	2.52	0.45
1:A:712:VAL:O	1:A:712:VAL:HG13	2.17	0.45
1:A:532:GLN:HE22	1:A:542:THR:C	2.20	0.45
1:A:116:TYR:HB3	1:A:123:LEU:HD11	1.99	0.44
1:A:155:ILE:HD12	1:A:158:ILE:CG2	2.47	0.44
1:A:726:VAL:HG13	1:A:727:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ASN:HA	5:A:2153:HOH:O	2.15	0.44
1:A:354:LEU:CD1	1:A:425:LEU:CD1	2.95	0.44
1:A:743:LYS:CE	5:A:2428:HOH:O	2.10	0.44
1:A:706:TYR:O	1:A:708:LEU:N	2.48	0.44
1:A:763:GLU:O	1:A:764:SER:HB3	2.18	0.44
1:A:419:ASP:O	1:A:423:LYS:HG3	2.18	0.44
1:A:118:TYR:CE2	1:A:153:PRO:HA	2.53	0.43
1:A:194:GLN:HG3	5:A:2141:HOH:O	2.17	0.43
1:A:283:GLN:NE2	1:A:327:THR:OG1	2.46	0.43
1:A:331:MET:CE	1:A:345:PHE:HZ	2.30	0.43
1:A:308:ASN:OD1	1:A:309:GLN:NE2	2.50	0.43
1:A:344:ILE:HD11	1:A:432:TRP:HZ3	1.83	0.43
1:A:759:GLU:HB3	1:A:760:GLN:OE1	2.18	0.43
1:A:49:CYS:SG	5:A:2051:HOH:O	2.62	0.43
1:A:701:PHE:HZ	1:A:727:LEU:HD11	1.83	0.43
1:A:744:ILE:O	1:A:744:ILE:HG23	2.19	0.43
1:A:282:TYR:CZ	1:A:307:LEU:HD22	2.54	0.43
1:A:750:GLN:HE22	1:A:753:ARG:NE	2.11	0.43
1:A:709:ALA:HA	1:A:729:HIS:HD2	1.80	0.42
1:A:35:ILE:HG21	1:A:62:PHE:CG	2.54	0.42
1:A:127:ASN:HB2	1:A:183:ALA:O	2.19	0.42
1:A:176:LEU:HD12	1:A:652:PHE:CE1	2.54	0.42
1:A:206:ASN:HB2	5:A:2153:HOH:O	2.19	0.42
1:A:285:LEU:HD11	1:A:307:LEU:HD11	1.98	0.42
1:A:354:LEU:CD1	1:A:425:LEU:HD11	2.49	0.42
1:A:473:TYR:CE2	1:A:638:LEU:HD23	2.53	0.42
1:A:581:ILE:O	1:A:582:GLN:C	2.58	0.42
1:A:736:GLN:OE1	1:A:747:ARG:HD2	2.19	0.42
1:A:767:PRO:CB	1:A:768:PRO:HD3	2.49	0.42
1:A:582:GLN:O	1:A:583:ASP:HB2	2.20	0.42
1:A:593:GLN:NE2	5:A:2373:HOH:O	2.52	0.42
1:A:745:PHE:N	1:A:745:PHE:CD2	2.88	0.42
1:A:379:SER:HB3	1:A:384:VAL:O	2.20	0.41
1:A:669:ASP:O	1:A:673:LEU:HG	2.20	0.41
1:A:727:LEU:HD23	1:A:737:TYR:CE2	2.55	0.41
1:A:43:GLU:CD	5:A:2040:HOH:O	2.58	0.41
1:A:294:LYS:HB2	5:A:2186:HOH:O	2.09	0.41
1:A:482:PHE:CZ	1:A:486:MET:HG3	2.55	0.41
1:A:610:LYS:CD	1:A:614:ASP:HB2	2.48	0.41
1:A:206:ASN:CB	5:A:2153:HOH:O	2.68	0.41
1:A:763:GLU:HG3	1:A:764:SER:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:VAL:HA	1:A:425:LEU:HD12	2.03	0.41
1:A:707:LEU:HD11	1:A:713:PRO:HG3	2.03	0.41
1:A:732:ILE:HG22	1:A:754:ILE:HG12	2.02	0.41
1:A:737:TYR:HE1	1:A:739:PHE:CE2	2.39	0.41
2:A:1778:H70:CE2	5:A:2268:HOH:O	2.53	0.41
1:A:622:LYS:HE2	1:A:622:LYS:HB3	1.88	0.41
1:A:3:PRO:HB2	1:A:142:ILE:CD1	2.51	0.40
1:A:520:ARG:HH11	1:A:520:ARG:HG2	1.87	0.40
1:A:715:ASP:O	1:A:716:ALA:HB2	2.21	0.40
1:A:761:ARG:CD	1:A:763:GLU:C	2.89	0.40
1:A:431:LEU:HB2	2:A:1778:H70:BR2	2.77	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:204:GLN:OE1	1:A:615:PRO:CB[3_754]	1.76	0.44

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	774/776 (100%)	717 (93%)	52 (7%)	5 (1%)	25 36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	714	ARG
1	A	208	SER
1	A	702	VAL
1	A	775	ILE
1	A	499	ILE

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	680/680 (100%)	667 (98%)	13 (2%)	57 75

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

Mol	Chain	Res	Type
1	A	12	HIS
1	A	70	ARG
1	A	147	ARG
1	A	196	LEU
1	A	211	LEU
1	A	216	LEU
1	A	322	GLU
1	A	412	GLU
1	A	602	ASP
1	A	611	LEU
1	A	659	ASN
1	A	694	ASN
1	A	695	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	104	HIS
1	A	112	GLN
1	A	154	HIS
1	A	172	ASN
1	A	188	ASN
1	A	194	GLN
1	A	227	ASN
1	A	283	GLN
1	A	353	HIS
1	A	408	HIS
1	A	475	ASN

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Mol	Chain	Res	Type
1	A	484	HIS
1	A	491	GLN
1	A	511	GLN
1	A	521	GLN
1	A	532	GLN
1	A	541	ASN
1	A	593	GLN
1	A	613	ASN
1	A	659	ASN
1	A	675	GLN
1	A	679	ASN
1	A	694	ASN
1	A	729	HIS
1	A	750	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)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\#\|Z\| > 2$
3	AD9	A	1779	4	24,33,33	2.01	6 (25%)	26,52,52	1.59	2 (7%)
2	H70	A	1778	-	13,18,18	2.31	7 (53%)	16,27,27	1.62	3 (18%)

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	AD9	A	1779	4	-	0/12/38/38	0/3/3/3
2	H70	A	1778	-	-	0/0/4/4	0/2/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1779	AD9	O3B-VG	6.66	2.10	1.80
3	A	1779	AD9	C2'-C3'	-3.97	1.42	1.53
2	A	1778	H70	C3-CE2	3.52	1.44	1.38
2	A	1778	H70	C9-C8	3.45	1.45	1.38
2	A	1778	H70	C3-CH	3.19	1.43	1.38
2	A	1778	H70	BR3-C7	-2.86	1.85	1.90
2	A	1778	H70	BR2-C8	-2.86	1.83	1.89
3	A	1779	AD9	C6-N6	2.66	1.43	1.34
3	A	1779	AD9	C3'-C4'	-2.50	1.46	1.53
3	A	1779	AD9	C2'-C1'	-2.49	1.50	1.53
3	A	1779	AD9	O5'-C5'	-2.26	1.36	1.44
2	A	1778	H70	CE2-CL1	-2.05	1.70	1.74
2	A	1778	H70	CD2-CE2	2.04	1.40	1.36

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1779	AD9	N3-C2-N1	-5.22	120.53	128.68
2	A	1778	H70	C7-C8-C9	3.24	107.16	104.48
3	A	1779	AD9	C2-N1-C6	3.13	124.11	118.75
2	A	1778	H70	O-CR-CG	2.94	122.88	116.64
2	A	1778	H70	CR-CH-CL2	2.36	121.73	118.79

There are no chirality outliers.

There are no torsion outliers.

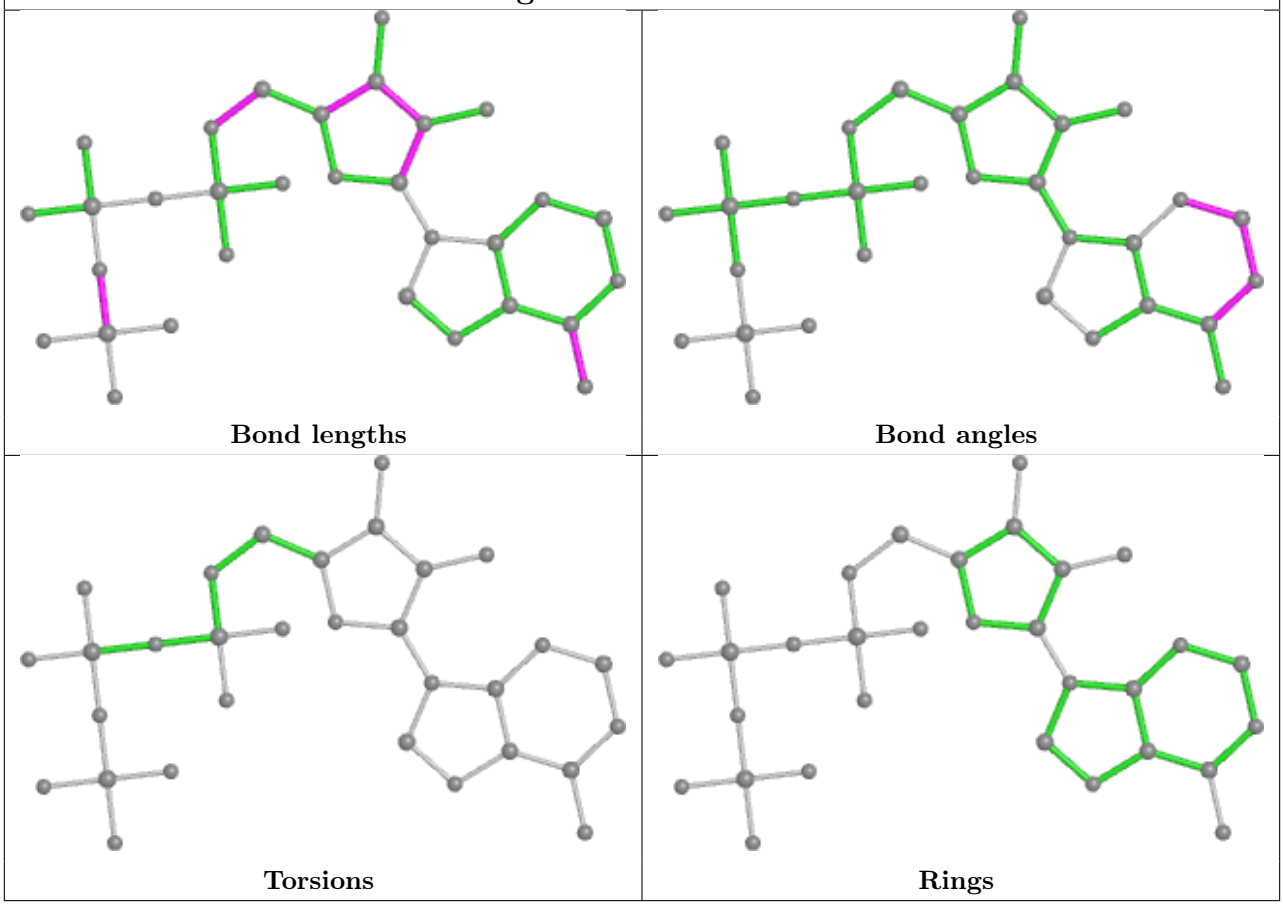
There are no ring outliers.

2 monomers are involved in 18 short contacts:

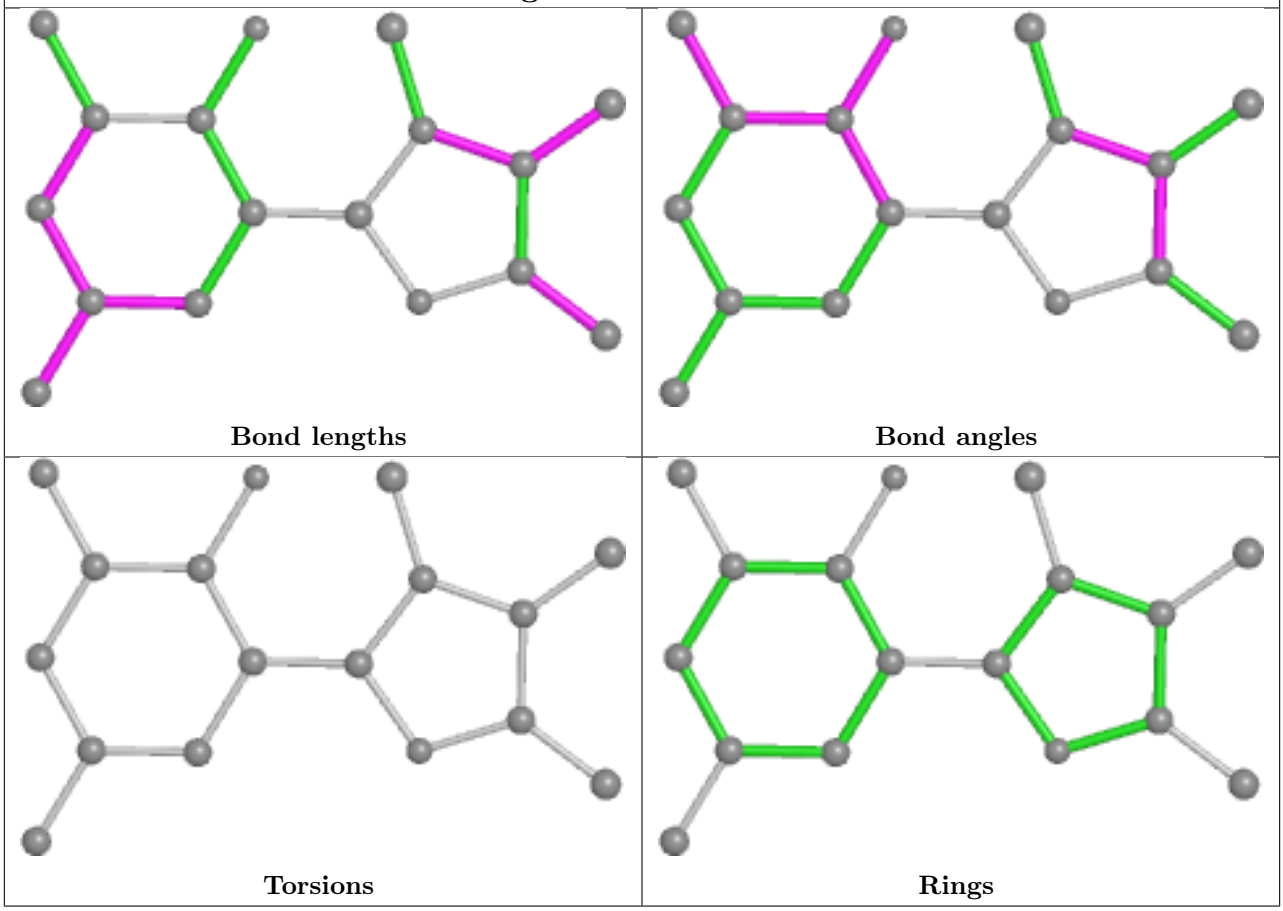
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1779	AD9	1	0
2	A	1778	H70	17	0

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 AD9 A 1779



Ligand H70 A 1778



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	776/776 (100%)	0.74	102 (13%) 3 3	23, 43, 123, 157	21 (2%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	777	PHE	16.5
1	A	771	PHE	16.4
1	A	757	ALA	15.8
1	A	756	GLU	13.9
1	A	754	ILE	13.0
1	A	770	ASP	12.0
1	A	711	ASN	11.8
1	A	776	PRO	11.3
1	A	705	TYR	11.1
1	A	775	ILE	10.9
1	A	207	GLY	10.7
1	A	767	PRO	10.5
1	A	760	GLN	9.9
1	A	766	GLU	9.6
1	A	774	ASP	9.4
1	A	752	ALA	9.1
1	A	729	HIS	9.1
1	A	758	ARG	8.9
1	A	731	ASN	8.6
1	A	734	PRO	8.4
1	A	772	ASP	8.3
1	A	764	SER	8.2
1	A	205	ALA	8.1
1	A	203	ASN	7.9
1	A	206	ASN	7.7
1	A	730	LEU	7.4
1	A	762	LEU	7.3

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Mol	Chain	Res	Type	RSRZ
1	A	773	ASP	7.3
1	A	765	ASN	7.2
1	A	712	VAL	7.2
1	A	759	GLU	7.0
1	A	713	PRO	7.0
1	A	769	MET	6.8
1	A	208	SER	6.7
1	A	753	ARG	6.2
1	A	204	GLN	6.2
1	A	720	GLN	5.9
1	A	706	TYR	5.9
1	A	709	ALA	5.8
1	A	761	ARG	5.6
1	A	701	PHE	5.3
1	A	722	ALA	5.2
1	A	763	GLU	5.2
1	A	707	LEU	5.1
1	A	768	PRO	5.1
1	A	755	GLU	4.6
1	A	704	ARG	4.5
1	A	699	ALA	4.4
1	A	735	GLU	4.4
1	A	732	ILE	4.4
1	A	698	TYR	4.4
1	A	710	PRO	4.0
1	A	745	PHE	3.8
1	A	393	LEU	3.7
1	A	718	ASP	3.5
1	A	714	ARG	3.4
1	A	744	ILE	3.3
1	A	290	ALA	3.3
1	A	291	GLU	3.3
1	A	737	TYR	3.2
1	A	733	ASP	3.2
1	A	719	SER	3.2
1	A	525	ILE	3.2
1	A	623	LYS	3.2
1	A	703	LYS	3.2
1	A	67	GLY	3.2
1	A	721	LYS	3.1
1	A	348	ILE	3.1
1	A	708	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	702	VAL	3.0
1	A	344	ILE	2.9
1	A	520	ARG	2.9
1	A	725	ALA	2.8
1	A	741	ILE	2.8
1	A	723	THR	2.8
1	A	717	GLU	2.7
1	A	626	ASN	2.7
1	A	66	ASP	2.6
1	A	746	PHE	2.6
1	A	502	THR	2.5
1	A	294	LYS	2.5
1	A	44	ARG	2.5
1	A	394	MET	2.5
1	A	728	LYS	2.4
1	A	363	ALA	2.4
1	A	716	ALA	2.4
1	A	170	ARG	2.4
1	A	742	THR	2.4
1	A	249	SER	2.3
1	A	736	GLN	2.3
1	A	364	GLY	2.3
1	A	625	ALA	2.3
1	A	748	ALA	2.3
1	A	738	ARG	2.2
1	A	280	ILE	2.2
1	A	715	ASP	2.2
1	A	727	LEU	2.2
1	A	496	LYS	2.2
1	A	365	GLU	2.2
1	A	65	VAL	2.1
1	A	102	VAL	2.1
1	A	692	PHE	2.1

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)

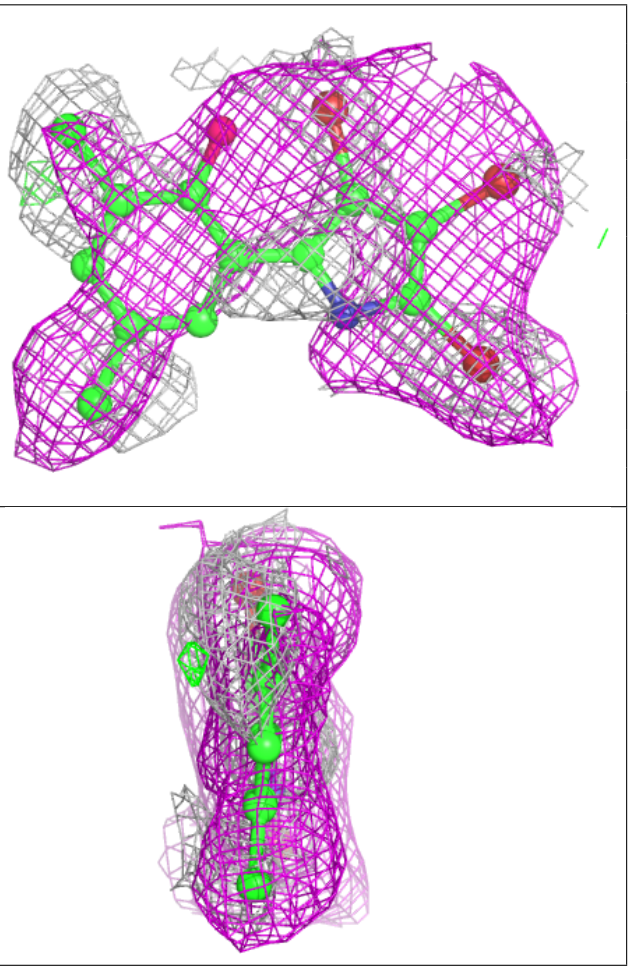
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	H70	A	1778	17/17	0.50	0.70	56,64,117,123	0
4	MG	A	1780	1/1	0.94	0.06	37,37,37,37	0
3	AD9	A	1779	31/31	0.97	0.12	24,29,33,34	0

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

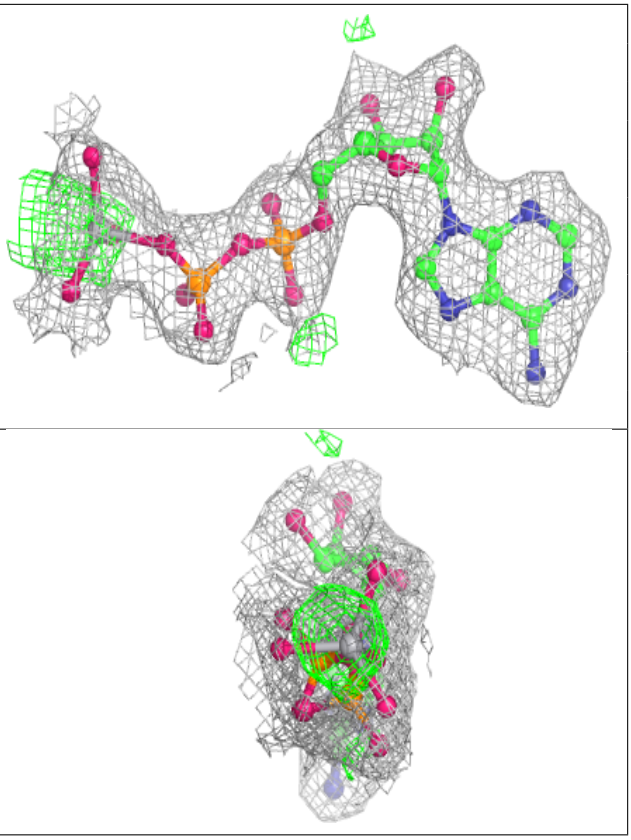
Electron density around H70 A 1778:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around AD9 A 1779:

$2mF_o$-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.