



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:44 PM UTC

PDB ID : 2JHR / pdb_00002jhr
Title : Crystal structure of myosin-2 motor domain in complex with ADP- metavana-
date and pentabromopseudilin
Authors : Fedorov, R.; Boehl, M.; Tsiavaliaris, G.; Hartmann, F.K.; Baruch, P.; Brenner,
B.; Martin, R.; Knoelker, H.J.; Gutzeit, H.O.; Manstein, D.J.
Deposited on : 2008-03-25
Resolution : 2.80 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

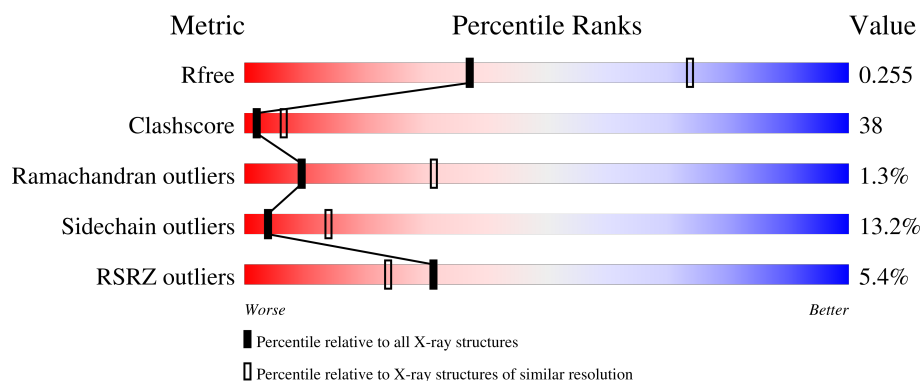
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 $\leq 5\%$. 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	788	

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
4	PBQ	A	1780	-	-	X	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6761 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	6239	3961	1076	1185	17	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

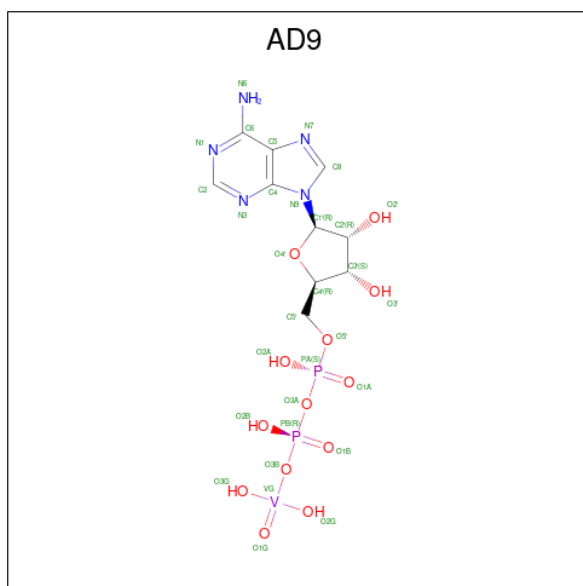
Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	expression tag	UNP P08799
A	-9	HIS	-	expression tag	UNP P08799
A	-8	HIS	-	expression tag	UNP P08799
A	-7	HIS	-	expression tag	UNP P08799
A	-6	HIS	-	expression tag	UNP P08799
A	-5	HIS	-	expression tag	UNP P08799
A	-4	HIS	-	expression tag	UNP P08799
A	-3	HIS	-	expression tag	UNP P08799
A	-2	ASP	-	expression tag	UNP P08799
A	-1	GLY	-	expression tag	UNP P08799
A	0	THR	-	expression tag	UNP P08799
A	1	GLU	-	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

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Chain	Residue	Modelled	Actual	Comment	Reference
A	777	PHE	-	expression tag	UNP P08799

- Molecule 2 is ADP METAVANADATE (CCD ID: AD9) (formula: $C_{10}H_{16}N_5O_{13}P_2V$).

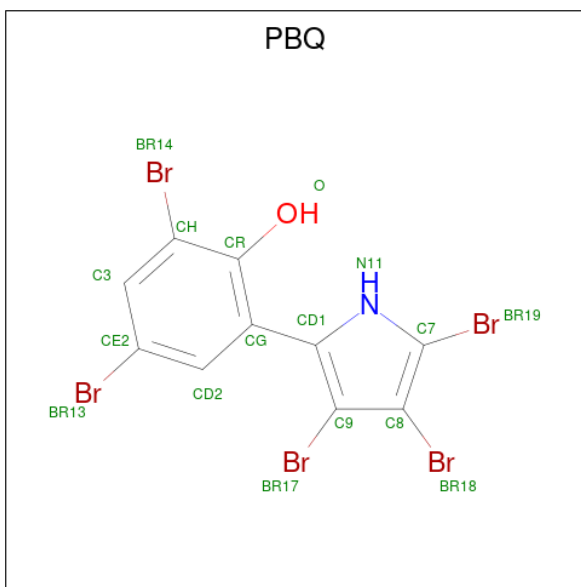


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P	V	
2	A	1	31	10	5	13	2	1	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is PENTABROMOPSEUDILIN (CCD ID: PBQ) (formula: $C_{10}H_4Br_5NO$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	Br	C	N	O	0	0
			17	5	10	1	1		

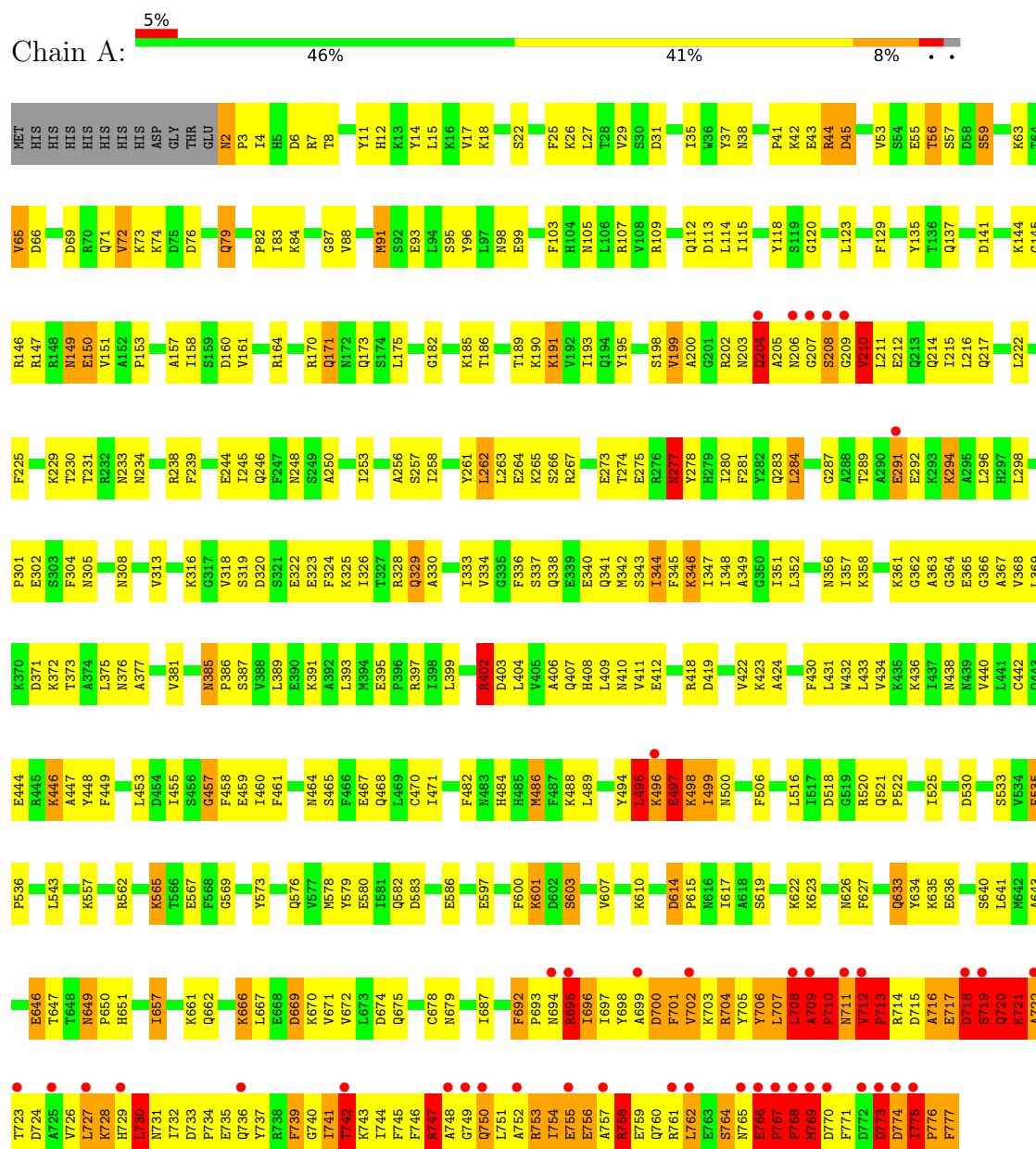
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	473	Total	O	0	0
			473	473		

3 Residue-property plots

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



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	89.76Å 150.46Å 154.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80 8.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.80) 77.3 (8.00-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.84 (at 2.20Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.217 , 0.265 0.218 , 0.255	Depositor DCC
R_{free} test set	9883 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtriage
Anisotropy	0.674	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 117.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.027 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	6761	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, PBQ, 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	0.68	5/6364 (0.1%)	1.35	88/8590 (1.0%)

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	10

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	713	PRO	N-CD	19.37	1.74	1.47
1	A	747	ARG	C-N	-12.78	1.16	1.33
1	A	718	ASP	C-N	-7.30	1.22	1.33
1	A	710	PRO	N-CD	7.09	1.57	1.47
1	A	767	PRO	N-CD	6.47	1.56	1.47

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	ASN	CB-CA-C	-20.58	78.87	112.00
1	A	739	PHE	CB-CA-C	-18.49	79.97	111.41
1	A	741	ILE	N-CA-C	18.44	147.70	109.34
1	A	711	ASN	N-CA-C	18.28	146.24	107.67
1	A	741	ILE	N-CA-CB	-17.26	82.75	111.23
1	A	495	LEU	N-CA-C	16.39	133.64	112.34
1	A	719	SER	N-CA-C	-15.18	92.38	114.39
1	A	711	ASN	CB-CA-C	-13.54	92.32	111.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	708	LEU	CB-CA-C	13.41	137.10	110.42
1	A	741	ILE	CB-CA-C	-13.11	89.80	111.29
1	A	365	GLU	N-CA-C	13.04	126.95	111.82
1	A	204	GLN	N-CA-C	12.85	138.18	110.80
1	A	708	LEU	N-CA-C	-12.80	83.54	110.80
1	A	757	ALA	CB-CA-C	12.80	130.97	110.88
1	A	747	ARG	CB-CA-C	-11.60	90.93	109.84
1	A	758	ARG	N-CA-CB	-11.18	95.14	110.67
1	A	747	ARG	O-C-N	-10.59	110.65	123.04
1	A	748	ALA	N-CA-CB	10.55	127.31	111.70
1	A	722	ALA	CB-CA-C	-10.13	89.50	110.17
1	A	742	THR	N-CA-C	-10.11	89.27	110.80
1	A	713	PRO	N-CA-CB	9.35	113.06	103.25
1	A	713	PRO	CA-N-CD	-9.31	98.97	112.00
1	A	718	ASP	N-CA-C	-9.21	91.17	110.80
1	A	713	PRO	N-CA-C	-9.05	93.83	112.47
1	A	719	SER	N-CA-CB	8.79	122.58	110.98
1	A	261	TYR	N-CA-C	8.50	123.78	108.48
1	A	718	ASP	CB-CA-C	8.47	127.27	110.42
1	A	365	GLU	CB-CA-C	-8.41	94.52	110.67
1	A	747	ARG	N-CA-C	8.29	122.94	109.76
1	A	718	ASP	O-C-N	-8.15	111.75	122.59
1	A	757	ALA	N-CA-C	-7.62	102.91	111.07
1	A	210	VAL	N-CA-C	-7.36	105.48	111.81
1	A	742	THR	N-CA-CB	7.20	122.66	110.49
1	A	709	ALA	N-CA-C	7.12	125.54	109.81
1	A	649	ASN	CA-C-N	6.76	127.29	119.99
1	A	649	ASN	C-N-CA	6.76	127.29	119.99
1	A	447	ALA	N-CA-C	-6.72	105.08	113.55
1	A	208	SER	N-CA-CB	-6.70	99.17	110.49
1	A	349	ALA	N-CA-C	-6.66	103.95	111.14
1	A	669	ASP	N-CA-C	6.50	120.42	112.23
1	A	750	GLN	N-CA-C	-6.50	104.04	112.23
1	A	494	TYR	CB-CA-C	-6.49	97.14	110.38
1	A	713	PRO	CB-CA-C	-6.45	100.91	111.56
1	A	767	PRO	N-CA-C	6.42	118.53	110.70
1	A	261	TYR	CB-CA-C	-6.41	98.90	109.80
1	A	712	VAL	N-CA-C	-6.29	95.29	108.88
1	A	729	HIS	N-CA-C	-6.29	104.43	111.28
1	A	535	PHE	CA-C-N	6.18	127.57	119.84
1	A	535	PHE	C-N-CA	6.18	127.57	119.84
1	A	735	GLU	N-CA-C	-6.09	105.83	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	657	ILE	N-CA-C	-6.04	103.44	108.63
1	A	486	MET	N-CA-C	6.02	117.93	111.36
1	A	712	VAL	C-N-CD	-5.97	100.52	125.00
1	A	601	LYS	N-CA-C	-5.93	104.89	111.71
1	A	775	ILE	N-CA-C	5.92	121.67	108.88
1	A	701	PHE	N-CA-C	-5.92	104.96	111.82
1	A	543	LEU	N-CA-C	5.87	117.48	111.14
1	A	338	GLN	N-CA-C	-5.80	105.70	112.89
1	A	346	LYS	N-CA-C	-5.79	105.05	111.36
1	A	614	ASP	CA-C-N	5.76	125.89	119.32
1	A	614	ASP	C-N-CA	5.76	125.89	119.32
1	A	45	ASP	N-CA-C	5.76	120.17	113.20
1	A	377	ALA	N-CA-C	-5.67	104.78	110.97
1	A	767	PRO	N-CA-CB	-5.67	97.58	103.08
1	A	204	GLN	N-CA-CB	-5.66	100.93	110.49
1	A	402	ARG	N-CA-C	-5.65	105.33	114.09
1	A	748	ALA	CB-CA-C	-5.63	103.89	111.89
1	A	363	ALA	N-CA-C	-5.59	105.27	111.36
1	A	2	ASN	CA-C-N	5.57	125.23	119.05
1	A	2	ASN	C-N-CA	5.57	125.23	119.05
1	A	262	LEU	N-CA-C	5.42	118.91	111.54
1	A	721	LYS	N-CA-C	-5.41	104.93	112.45
1	A	650	PRO	N-CA-C	5.37	120.50	111.32
1	A	457	GLY	N-CA-C	5.36	120.71	112.51
1	A	767	PRO	CA-N-CD	-5.33	104.54	112.00
1	A	695	ARG	N-CA-C	5.32	117.04	108.32
1	A	748	ALA	N-CA-C	5.30	118.70	111.39
1	A	277	ASN	N-CA-C	-5.29	101.51	109.60
1	A	364	GLY	N-CA-C	-5.28	105.33	112.57
1	A	385	ASN	CA-C-N	5.26	126.41	119.84
1	A	385	ASN	C-N-CA	5.26	126.41	119.84
1	A	730	LEU	N-CA-C	-5.20	106.71	113.16
1	A	710	PRO	CA-N-CD	-5.17	104.76	112.00
1	A	720	GLN	N-CA-C	-5.07	107.04	113.18
1	A	364	GLY	CA-C-N	5.04	127.97	120.31
1	A	364	GLY	C-N-CA	5.04	127.97	120.31
1	A	55	GLU	N-CA-C	5.03	115.17	108.38
1	A	59	SER	N-CA-C	5.01	116.69	109.07

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	711	ASN	Peptide
1	A	712	VAL	Peptide
1	A	718	ASP	Mainchain
1	A	747	ARG	Mainchain
1	A	767	PRO	Peptide
1	A	768	PRO	Peptide
1	A	769	MET	Peptide
1	A	773	ASP	Peptide
1	A	775	ILE	Peptide
1	A	776	PRO	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	6239	0	6175	473	0
2	A	31	0	14	2	0
3	A	1	0	0	0	0
4	A	17	0	3	11	0
5	A	473	0	0	35	0
All	All	6761	0	6192	476	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 38.

All (476) 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:713:PRO:N	1:A:713:PRO:CD	1.74	1.44
1:A:431:LEU:HD13	4:A:1780:PBQ:BR18	1.95	1.20
1:A:773:ASP:H	1:A:775:ILE:HG22	1.10	1.16
1:A:496:LYS:O	1:A:498:LYS:HG2	1.47	1.12
1:A:739:PHE:HA	1:A:744:ILE:HG13	1.31	1.12
1:A:202:ARG:HB2	1:A:208:SER:HB3	1.34	1.09
1:A:424:ALA:HB2	4:A:1780:PBQ:BR14	2.07	1.09
1:A:767:PRO:HD2	1:A:768:PRO:CD	1.83	1.08
1:A:204:GLN:HA	1:A:209:GLY:HA3	1.25	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:767:PRO:HD2	1:A:768:PRO:HD2	1.03	1.02
1:A:204:GLN:CA	1:A:209:GLY:HA3	1.88	1.01
1:A:499:ILE:HD12	1:A:740:GLY:HA3	1.42	1.00
1:A:206:ASN:HA	1:A:210:VAL:HB	1.43	1.00
1:A:736:GLN:OE1	1:A:747:ARG:HB2	1.62	0.98
1:A:756:GLU:HA	1:A:759:GLU:HB3	1.41	0.97
1:A:712:VAL:C	1:A:713:PRO:CD	2.38	0.97
1:A:766:GLU:H	1:A:767:PRO:HD3	1.30	0.94
1:A:767:PRO:CD	1:A:768:PRO:HD2	1.95	0.93
1:A:173:GLN:HE22	1:A:649:ASN:HD22	1.00	0.93
1:A:766:GLU:N	1:A:767:PRO:HD3	1.82	0.92
1:A:204:GLN:HA	1:A:209:GLY:CA	1.99	0.92
1:A:277:ASN:HD22	1:A:278:TYR:H	1.18	0.92
1:A:740:GLY:O	1:A:743:LYS:O	1.90	0.90
1:A:366:GLY:HA3	1:A:408:HIS:ND1	1.89	0.87
1:A:366:GLY:HA3	1:A:408:HIS:CE1	2.09	0.86
1:A:712:VAL:CG1	1:A:712:VAL:O	2.25	0.85
1:A:773:ASP:N	1:A:775:ILE:HG22	1.92	0.85
1:A:712:VAL:N	1:A:713:PRO:HD3	1.91	0.85
1:A:741:ILE:HG23	1:A:741:ILE:O	1.77	0.84
1:A:325:LYS:O	1:A:329:GLN:HG2	1.78	0.84
1:A:610:LYS:HE3	1:A:614:ASP:HB2	1.59	0.83
1:A:262:LEU:HD11	1:A:470:CYS:HB3	1.60	0.83
1:A:712:VAL:CA	1:A:713:PRO:HD3	2.09	0.83
1:A:569:GLY:HA3	1:A:578:MET:HE2	1.61	0.83
1:A:707:LEU:O	1:A:708:LEU:C	2.22	0.82
1:A:461:PHE:H	1:A:464:ASN:HD21	1.27	0.82
1:A:712:VAL:O	1:A:712:VAL:HG13	1.80	0.81
1:A:712:VAL:CA	1:A:713:PRO:CD	2.59	0.81
1:A:764:SER:HA	1:A:768:PRO:HD3	1.62	0.81
1:A:727:LEU:HD12	1:A:732:ILE:HD11	1.62	0.81
1:A:741:ILE:O	1:A:741:ILE:CG2	2.23	0.80
1:A:53:VAL:HG21	1:A:63:LYS:HG3	1.61	0.80
1:A:497:GLU:HG2	1:A:745:PHE:HE2	1.47	0.79
1:A:766:GLU:N	1:A:767:PRO:CD	2.46	0.79
1:A:697:ILE:HD12	1:A:697:ILE:H	1.47	0.79
1:A:750:GLN:HA	1:A:753:ARG:HH11	1.47	0.79
1:A:707:LEU:C	1:A:708:LEU:O	2.06	0.78
1:A:719:SER:O	1:A:723:THR:HG23	1.84	0.78
1:A:329:GLN:HE21	1:A:329:GLN:HA	1.49	0.78
1:A:173:GLN:HE22	1:A:649:ASN:ND2	1.80	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:746:PHE:HD2	1:A:751:LEU:HB2	1.51	0.76
1:A:760:GLN:HG3	5:A:2209:HOH:O	1.84	0.76
1:A:465:SER:H	1:A:468:GLN:NE2	1.82	0.76
1:A:761:ARG:O	1:A:765:ASN:HB2	1.85	0.76
1:A:239:PHE:HB3	1:A:263:LEU:HD12	1.68	0.75
1:A:424:ALA:HA	4:A:1780:PBQ:O	1.85	0.75
1:A:695:ARG:HH11	1:A:695:ARG:HB3	1.51	0.75
1:A:262:LEU:HD23	1:A:262:LEU:O	1.86	0.75
1:A:773:ASP:H	1:A:775:ILE:CG2	1.96	0.74
1:A:431:LEU:CD1	4:A:1780:PBQ:BR18	2.86	0.74
4:A:1780:PBQ:BR17	4:A:1780:PBQ:HD2	2.43	0.74
1:A:145:GLY:H	1:A:164:ARG:HH21	1.37	0.73
1:A:617:ILE:O	4:A:1780:PBQ:BR17	2.61	0.73
1:A:718:ASP:O	1:A:721:LYS:HE2	1.89	0.73
1:A:424:ALA:CB	4:A:1780:PBQ:BR14	2.91	0.72
1:A:693:PRO:HA	1:A:695:ARG:HH22	1.55	0.72
1:A:246:GLN:HG2	1:A:446:LYS:HB3	1.72	0.71
1:A:706:TYR:H	1:A:706:TYR:HD2	1.38	0.71
1:A:706:TYR:N	1:A:706:TYR:CD2	2.58	0.71
1:A:706:TYR:O	1:A:712:VAL:HG13	1.91	0.71
1:A:461:PHE:N	1:A:464:ASN:HD21	1.88	0.71
1:A:453:LEU:HD13	1:A:641:LEU:HD21	1.73	0.70
1:A:25:PHE:O	1:A:29:VAL:HG22	1.92	0.70
1:A:755:GLU:O	1:A:758:ARG:HG3	1.90	0.70
1:A:762:LEU:O	1:A:767:PRO:HG3	1.92	0.69
1:A:118:TYR:CD2	1:A:153:PRO:HG3	2.27	0.69
1:A:753:ARG:HA	1:A:756:GLU:OE1	1.92	0.69
1:A:694:ASN:HB2	1:A:746:PHE:HB2	1.73	0.69
1:A:186:THR:O	1:A:190:LYS:HG3	1.92	0.69
1:A:736:GLN:CD	1:A:747:ARG:HB2	2.17	0.69
1:A:305:ASN:H	1:A:356:ASN:HD21	1.41	0.69
1:A:736:GLN:OE1	1:A:750:GLN:HB2	1.92	0.68
1:A:695:ARG:HB2	1:A:743:LYS:HD2	1.75	0.68
1:A:347:ILE:O	1:A:351:ILE:HG13	1.93	0.68
1:A:291:GLU:O	1:A:294:LYS:HG3	1.93	0.68
1:A:265:LYS:HD3	4:A:1780:PBQ:BR19	2.48	0.68
1:A:499:ILE:HD12	1:A:740:GLY:CA	2.23	0.68
1:A:615:PRO:O	1:A:619:SER:HB2	1.93	0.68
1:A:727:LEU:HD23	1:A:728:LYS:N	2.09	0.68
1:A:395:GLU:HA	1:A:407:GLN:O	1.94	0.67
1:A:14:TYR:HA	5:A:2024:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:GLN:HG3	1:A:209:GLY:HA3	1.77	0.67
1:A:693:PRO:HA	1:A:695:ARG:NH2	2.09	0.67
1:A:741:ILE:HG22	1:A:742:THR:HG22	1.77	0.67
1:A:329:GLN:O	1:A:333:ILE:HD13	1.95	0.67
1:A:499:ILE:HD11	1:A:740:GLY:H	1.59	0.67
1:A:773:ASP:O	1:A:776:PRO:CG	2.43	0.67
1:A:775:ILE:HG23	1:A:776:PRO:CD	2.25	0.66
1:A:170:ARG:HG2	1:A:170:ARG:HH21	1.59	0.66
1:A:497:GLU:HG2	1:A:745:PHE:CE2	2.31	0.66
1:A:769:MET:HG2	1:A:770:ASP:OD1	1.94	0.66
1:A:773:ASP:HB2	1:A:775:ILE:H	1.60	0.66
1:A:775:ILE:HG23	1:A:776:PRO:HD3	1.78	0.66
1:A:767:PRO:CD	1:A:768:PRO:CD	2.65	0.65
1:A:206:ASN:CA	1:A:210:VAL:HB	2.23	0.65
1:A:773:ASP:O	1:A:776:PRO:HG2	1.97	0.65
1:A:764:SER:HA	1:A:768:PRO:CD	2.26	0.65
1:A:716:ALA:HB1	1:A:721:LYS:HE2	1.79	0.65
1:A:316:LYS:HB3	5:A:2200:HOH:O	1.97	0.65
1:A:704:ARG:O	1:A:758:ARG:NH1	2.29	0.65
1:A:708:LEU:HD21	1:A:758:ARG:HD2	1.78	0.64
1:A:375:LEU:HD12	1:A:389:LEU:HD23	1.80	0.64
1:A:706:TYR:O	1:A:712:VAL:O	2.15	0.64
1:A:580:GLU:HG3	5:A:2394:HOH:O	1.98	0.64
1:A:257:SER:HB3	1:A:442:CYS:SG	2.38	0.63
2:A:1778:AD9:O2A	5:A:2472:HOH:O	2.16	0.63
1:A:144:LYS:HG3	1:A:199:VAL:HG22	1.81	0.63
1:A:465:SER:H	1:A:468:GLN:HE21	1.46	0.63
1:A:597:GLU:O	1:A:601:LYS:HG3	1.99	0.63
1:A:273:GLU:O	1:A:274:THR:OG1	2.10	0.62
1:A:337:SER:HB2	1:A:340:GLU:HG3	1.81	0.62
1:A:323:GLU:OE1	1:A:326:ILE:HD12	1.98	0.62
1:A:145:GLY:N	1:A:164:ARG:HH21	1.97	0.62
1:A:761:ARG:O	1:A:761:ARG:HD2	1.99	0.62
1:A:697:ILE:HD12	1:A:697:ILE:N	2.14	0.62
1:A:728:LYS:C	1:A:731:ASN:H	2.08	0.62
1:A:144:LYS:HA	1:A:195:TYR:OH	2.00	0.61
1:A:351:ILE:HG23	1:A:422:VAL:HG13	1.80	0.61
1:A:727:LEU:HB2	1:A:732:ILE:HG12	1.83	0.61
1:A:202:ARG:HB3	5:A:2184:HOH:O	2.00	0.61
1:A:657:ILE:HG22	1:A:675:GLN:NE2	2.15	0.61
1:A:496:LYS:O	1:A:498:LYS:CG	2.37	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:THR:O	1:A:727:LEU:HD22	2.00	0.61
1:A:496:LYS:C	1:A:498:LYS:N	2.56	0.61
1:A:727:LEU:HD23	1:A:728:LYS:H	1.64	0.61
1:A:724:ASP:HA	1:A:727:LEU:HD21	1.83	0.60
1:A:210:VAL:O	1:A:214:GLN:HG3	2.01	0.60
1:A:305:ASN:H	1:A:356:ASN:ND2	1.99	0.60
1:A:497:GLU:CD	1:A:742:THR:HG23	2.27	0.60
1:A:193:ILE:HD12	1:A:245:ILE:HD11	1.83	0.60
1:A:239:PHE:HB3	1:A:263:LEU:CD1	2.30	0.60
1:A:761:ARG:HH11	1:A:765:ASN:HA	1.66	0.60
1:A:412:GLU:HB2	5:A:2284:HOH:O	2.02	0.60
1:A:721:LYS:HG2	1:A:722:ALA:N	2.14	0.60
1:A:4:ILE:HD12	1:A:146:ARG:NH2	2.17	0.59
1:A:211:LEU:O	1:A:215:ILE:HG13	2.00	0.59
1:A:495:LEU:C	1:A:496:LYS:HE2	2.27	0.59
1:A:708:LEU:HD11	1:A:758:ARG:CB	2.32	0.59
2:A:1778:AD9:O1G	2:A:1778:AD9:VG	1.59	0.59
1:A:63:LYS:HG2	1:A:69:ASP:CG	2.28	0.59
1:A:273:GLU:HG2	1:A:274:THR:HG23	1.84	0.59
1:A:230:THR:HA	1:A:275:GLU:CD	2.27	0.59
1:A:246:GLN:HG2	1:A:446:LYS:HD2	1.85	0.59
1:A:329:GLN:HE21	1:A:329:GLN:CA	2.16	0.58
1:A:458:PHE:HE1	1:A:460:ILE:HD11	1.67	0.58
1:A:758:ARG:HE	1:A:758:ARG:C	2.11	0.58
1:A:430:PHE:O	1:A:434:VAL:HG23	2.02	0.58
1:A:302:GLU:HA	1:A:308:ASN:HB3	1.85	0.58
1:A:45:ASP:OD1	1:A:670:LYS:HD2	2.02	0.58
1:A:696:ILE:HD11	1:A:746:PHE:CE2	2.39	0.58
1:A:202:ARG:HB2	1:A:208:SER:CB	2.22	0.58
1:A:361:LYS:HE3	1:A:362:GLY:O	2.04	0.58
1:A:438:ASN:O	1:A:442:CYS:HB2	2.03	0.58
1:A:565:LYS:HB2	1:A:565:LYS:NZ	2.19	0.58
1:A:397:ARG:HG2	1:A:397:ARG:HH11	1.69	0.57
1:A:499:ILE:CD1	1:A:740:GLY:HA3	2.27	0.57
1:A:93:GLU:HB3	5:A:2098:HOH:O	2.04	0.57
1:A:170:ARG:HG2	1:A:170:ARG:NH2	2.16	0.57
1:A:217:GLN:O	1:A:330:ALA:HB1	2.03	0.57
1:A:262:LEU:HD11	1:A:470:CYS:CB	2.34	0.57
1:A:753:ARG:HB2	5:A:2465:HOH:O	2.05	0.57
1:A:775:ILE:CG2	1:A:776:PRO:CD	2.81	0.57
1:A:766:GLU:O	1:A:766:GLU:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:LEU:CD1	1:A:389:LEU:HD23	2.35	0.57
1:A:720:GLN:O	1:A:720:GLN:HG3	2.05	0.57
1:A:708:LEU:HD11	1:A:758:ARG:HB3	1.86	0.56
1:A:281:PHE:CD1	1:A:352:LEU:HD21	2.40	0.56
1:A:761:ARG:HD2	1:A:765:ASN:HB2	1.88	0.56
1:A:741:ILE:HG22	1:A:742:THR:N	2.02	0.56
1:A:701:PHE:CE2	1:A:723:THR:HG22	2.41	0.56
1:A:736:GLN:O	1:A:747:ARG:HG3	2.06	0.56
1:A:761:ARG:O	1:A:765:ASN:CB	2.53	0.56
1:A:341:GLN:O	1:A:344:ILE:HB	2.06	0.55
1:A:765:ASN:OD1	1:A:765:ASN:C	2.49	0.55
1:A:231:THR:HG23	1:A:275:GLU:OE2	2.06	0.55
1:A:495:LEU:N	1:A:495:LEU:CD1	2.67	0.55
1:A:764:SER:C	1:A:767:PRO:HD2	2.31	0.55
1:A:432:TRP:NE1	1:A:436:LYS:HD3	2.22	0.55
1:A:495:LEU:N	1:A:495:LEU:HD13	2.22	0.55
1:A:697:ILE:HG13	1:A:743:LYS:HB3	1.88	0.55
1:A:775:ILE:O	1:A:775:ILE:HG13	2.06	0.55
1:A:79:GLN:HG2	1:A:96:TYR:CE2	2.41	0.55
1:A:728:LYS:HA	5:A:2462:HOH:O	2.05	0.55
1:A:135:TYR:CG	1:A:191:LYS:HD2	2.41	0.55
1:A:173:GLN:NE2	1:A:649:ASN:HB3	2.21	0.55
1:A:342:MET:HG3	1:A:346:LYS:HE3	1.89	0.55
1:A:499:ILE:O	1:A:500:ASN:HB2	2.05	0.55
1:A:697:ILE:HG23	1:A:742:THR:O	2.06	0.55
1:A:702:VAL:CG2	1:A:714:ARG:HG3	2.36	0.55
1:A:773:ASP:C	1:A:776:PRO:HD2	2.32	0.55
1:A:697:ILE:HG22	1:A:698:TYR:N	2.22	0.55
1:A:707:LEU:O	1:A:708:LEU:O	2.24	0.55
1:A:724:ASP:O	1:A:728:LYS:HB3	2.06	0.55
1:A:633:GLN:O	1:A:636:GLU:HB3	2.07	0.55
1:A:708:LEU:HD21	1:A:758:ARG:HB2	1.88	0.54
1:A:646:GLU:OE1	1:A:646:GLU:HA	2.06	0.54
1:A:746:PHE:CD2	1:A:751:LEU:HB2	2.36	0.54
1:A:157:ALA:O	1:A:161:VAL:HG23	2.07	0.54
1:A:402:ARG:HG2	1:A:402:ARG:HH11	1.73	0.54
1:A:497:GLU:OE2	1:A:742:THR:HG23	2.07	0.54
1:A:761:ARG:HB2	5:A:2466:HOH:O	2.07	0.54
1:A:701:PHE:CE2	1:A:723:THR:HA	2.43	0.54
1:A:107:ARG:HD3	5:A:2109:HOH:O	2.07	0.54
1:A:324:PHE:HE2	1:A:328:ARG:HH21	1.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:GLN:NE2	1:A:141:ASP:OD1	2.41	0.54
1:A:766:GLU:H	1:A:767:PRO:CD	2.08	0.54
1:A:291:GLU:HA	1:A:294:LYS:HZ3	1.72	0.53
1:A:657:ILE:HG22	1:A:675:GLN:HE22	1.74	0.53
1:A:399:LEU:HA	1:A:403:ASP:O	2.08	0.53
1:A:129:PHE:CZ	1:A:662:GLN:HA	2.43	0.53
1:A:147:ARG:HB2	1:A:150:GLU:CD	2.33	0.53
1:A:63:LYS:HG2	1:A:69:ASP:OD1	2.08	0.53
1:A:118:TYR:CE2	1:A:153:PRO:HG3	2.43	0.53
1:A:500:ASN:HB3	5:A:2324:HOH:O	2.06	0.53
1:A:455:ILE:HG12	5:A:2162:HOH:O	2.09	0.53
1:A:741:ILE:HG22	1:A:742:THR:CG2	2.39	0.53
1:A:11:TYR:CD2	1:A:15:LEU:HD12	2.44	0.53
1:A:326:ILE:HG23	5:A:2247:HOH:O	2.08	0.53
1:A:371:ASP:OD2	1:A:373:THR:HG23	2.09	0.53
1:A:758:ARG:O	1:A:761:ARG:HB3	2.09	0.53
1:A:6:ASP:OD1	1:A:8:THR:HB	2.09	0.53
1:A:727:LEU:HA	1:A:730:LEU:CD1	2.39	0.53
1:A:262:LEU:CD1	1:A:470:CYS:HB3	2.36	0.52
1:A:204:GLN:HG3	1:A:209:GLY:CA	2.39	0.52
1:A:397:ARG:HB3	1:A:404:LEU:HD11	1.91	0.52
1:A:357:ILE:HB	1:A:418:ARG:NH1	2.24	0.52
1:A:706:TYR:CD2	1:A:707:LEU:N	2.74	0.52
1:A:484:HIS:CE1	1:A:489:LEU:HD21	2.44	0.52
1:A:497:GLU:OE1	1:A:742:THR:HG23	2.09	0.52
1:A:112:GLN:O	1:A:113:ASP:HB2	2.10	0.52
1:A:694:ASN:CB	1:A:746:PHE:HB2	2.39	0.52
1:A:695:ARG:HH11	1:A:695:ARG:CB	2.22	0.52
1:A:225:PHE:CE2	1:A:280:ILE:HG12	2.44	0.52
1:A:200:ALA:O	1:A:253:ILE:HG12	2.09	0.52
1:A:419:ASP:O	1:A:423:LYS:HG3	2.10	0.52
1:A:175:LEU:HD12	1:A:651:HIS:HB2	1.91	0.52
1:A:367:ALA:HB2	1:A:411:VAL:N	2.25	0.52
1:A:635:LYS:HE2	5:A:2340:HOH:O	2.09	0.52
1:A:461:PHE:H	1:A:464:ASN:ND2	2.04	0.51
1:A:622:LYS:HA	1:A:627:PHE:HA	1.90	0.51
1:A:144:LYS:HG3	1:A:199:VAL:CG2	2.40	0.51
1:A:147:ARG:HB2	1:A:150:GLU:CG	2.41	0.51
1:A:750:GLN:HG2	1:A:754:ILE:HD12	1.93	0.51
1:A:714:ARG:O	1:A:714:ARG:HG2	2.10	0.51
1:A:291:GLU:O	1:A:294:LYS:HE2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ALA:O	1:A:334:VAL:HG23	2.11	0.51
1:A:674:ASP:HB2	5:A:2448:HOH:O	2.11	0.51
1:A:699:ALA:O	1:A:702:VAL:HG13	2.11	0.51
1:A:715:ASP:O	1:A:716:ALA:HB2	2.09	0.51
1:A:698:TYR:HE1	1:A:744:ILE:HB	1.75	0.51
1:A:736:GLN:CD	1:A:750:GLN:HB2	2.36	0.51
1:A:56:THR:O	1:A:74:LYS:HE3	2.11	0.51
1:A:289:THR:OG1	1:A:292:GLU:HG3	2.11	0.51
1:A:79:GLN:HG2	1:A:96:TYR:CZ	2.46	0.50
1:A:244:GLU:HG3	1:A:449:PHE:CD2	2.47	0.50
1:A:506:PHE:CZ	1:A:687:ILE:HD13	2.47	0.50
1:A:764:SER:O	1:A:768:PRO:HD2	2.12	0.50
1:A:8:THR:HA	5:A:2007:HOH:O	2.10	0.50
1:A:135:TYR:CD1	1:A:191:LYS:HD2	2.47	0.50
1:A:516:LEU:O	1:A:525:ILE:HG13	2.12	0.50
1:A:727:LEU:HB2	1:A:732:ILE:CG1	2.41	0.50
1:A:751:LEU:O	1:A:755:GLU:HB2	2.11	0.50
1:A:701:PHE:HE2	1:A:723:THR:HG22	1.76	0.50
1:A:773:ASP:CB	1:A:775:ILE:H	2.24	0.50
1:A:53:VAL:CG2	1:A:63:LYS:HG3	2.38	0.50
1:A:280:ILE:HG13	1:A:348:ILE:HD13	1.92	0.50
1:A:496:LYS:C	1:A:498:LYS:H	2.20	0.50
1:A:601:LYS:HD3	5:A:2414:HOH:O	2.11	0.50
1:A:499:ILE:O	1:A:499:ILE:HG23	2.10	0.50
1:A:535:PHE:HD2	1:A:536:PRO:HD2	1.77	0.50
1:A:245:ILE:O	1:A:449:PHE:HA	2.12	0.49
1:A:334:VAL:HG12	1:A:440:VAL:HG21	1.93	0.49
1:A:369:LEU:HD23	1:A:375:LEU:HD22	1.94	0.49
1:A:76:ASP:HB3	5:A:2082:HOH:O	2.12	0.49
1:A:225:PHE:CE2	1:A:348:ILE:HD11	2.47	0.49
1:A:622:LYS:HG2	1:A:626:ASN:O	2.12	0.49
1:A:697:ILE:H	1:A:697:ILE:CD1	2.20	0.49
1:A:700:ASP:HA	1:A:703:LYS:HG2	1.93	0.49
1:A:701:PHE:HE2	1:A:723:THR:HA	1.78	0.49
1:A:708:LEU:HD13	5:A:2469:HOH:O	2.13	0.49
1:A:718:ASP:HB3	1:A:721:LYS:HD3	1.93	0.49
1:A:244:GLU:O	1:A:256:ALA:HA	2.12	0.49
1:A:323:GLU:OE1	1:A:323:GLU:HA	2.12	0.49
1:A:84:LYS:HG2	5:A:2095:HOH:O	2.13	0.49
1:A:120:GLY:HA3	5:A:2456:HOH:O	2.12	0.49
1:A:720:GLN:O	1:A:723:THR:OG1	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:SER:O	1:A:26:LYS:HG2	2.13	0.49
1:A:173:GLN:NE2	1:A:649:ASN:HD22	1.85	0.49
1:A:482:PHE:CE1	1:A:486:MET:HG3	2.48	0.49
1:A:712:VAL:N	1:A:713:PRO:CD	2.72	0.49
1:A:319:SER:HB3	1:A:322:GLU:HB2	1.94	0.49
1:A:557:LYS:HE3	5:A:2336:HOH:O	2.13	0.49
1:A:774:ASP:O	1:A:776:PRO:O	2.30	0.49
1:A:737:TYR:HB3	1:A:750:GLN:OE1	2.13	0.48
1:A:567:GLU:HA	1:A:579:TYR:O	2.13	0.48
1:A:737:TYR:HB2	1:A:745:PHE:O	2.13	0.48
1:A:752:ALA:HA	1:A:755:GLU:HB2	1.94	0.48
1:A:770:ASP:O	1:A:773:ASP:OD1	2.31	0.48
1:A:37:TYR:OH	1:A:65:VAL:HG22	2.13	0.48
1:A:482:PHE:CZ	1:A:486:MET:HG3	2.48	0.48
1:A:698:TYR:CE1	1:A:744:ILE:HB	2.47	0.48
1:A:44:ARG:NH1	1:A:99:GLU:OE2	2.47	0.48
1:A:518:ASP:HB2	1:A:635:LYS:HD2	1.95	0.48
1:A:692:PHE:HB2	1:A:745:PHE:HB3	1.94	0.48
1:A:277:ASN:ND2	1:A:278:TYR:H	1.99	0.48
1:A:432:TRP:CE2	1:A:436:LYS:HD3	2.49	0.48
1:A:204:GLN:HA	1:A:209:GLY:N	2.29	0.48
1:A:732:ILE:O	1:A:732:ILE:HG13	2.14	0.48
1:A:712:VAL:O	1:A:712:VAL:HG12	2.11	0.48
1:A:764:SER:C	1:A:768:PRO:HD2	2.39	0.48
1:A:734:PRO:HA	1:A:737:TYR:CE2	2.49	0.47
1:A:736:GLN:OE1	1:A:750:GLN:CB	2.61	0.47
1:A:776:PRO:O	1:A:777:PHE:C	2.57	0.47
1:A:206:ASN:OD1	1:A:206:ASN:O	2.32	0.47
1:A:728:LYS:O	1:A:731:ASN:ND2	2.47	0.47
1:A:222:LEU:HD11	1:A:258:ILE:HD13	1.96	0.47
1:A:98:ASN:HB3	5:A:2100:HOH:O	2.14	0.47
1:A:246:GLN:HG2	1:A:446:LYS:CD	2.44	0.47
1:A:372:LYS:HB2	1:A:376:ASN:HD21	1.79	0.47
1:A:698:TYR:HB3	1:A:719:SER:HB2	1.96	0.47
1:A:700:ASP:CA	1:A:703:LYS:HG2	2.44	0.47
1:A:700:ASP:O	1:A:703:LYS:HG2	2.15	0.46
1:A:724:ASP:HA	1:A:727:LEU:CD2	2.45	0.46
1:A:171:GLN:HE22	1:A:649:ASN:N	2.13	0.46
1:A:318:VAL:HG11	5:A:2083:HOH:O	2.15	0.46
1:A:573:TYR:O	1:A:678:CYS:HB2	2.15	0.46
1:A:582:GLN:O	1:A:583:ASP:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:ASP:OD1	5:A:2151:HOH:O	2.21	0.46
1:A:465:SER:N	1:A:468:GLN:HE21	2.11	0.46
1:A:225:PHE:CD2	1:A:280:ILE:HG12	2.51	0.46
1:A:248:ASN:HD21	1:A:250:ALA:HB3	1.81	0.46
1:A:264:GLU:O	1:A:278:TYR:OH	2.29	0.46
1:A:366:GLY:CA	1:A:408:HIS:CE1	2.91	0.46
1:A:385:ASN:HA	1:A:386:PRO:HD2	1.74	0.46
1:A:397:ARG:HA	1:A:406:ALA:HA	1.97	0.46
1:A:610:LYS:HE3	1:A:614:ASP:CB	2.38	0.46
1:A:705:TYR:CZ	1:A:754:ILE:HG22	2.50	0.46
1:A:137:GLN:HE21	1:A:141:ASP:CG	2.24	0.46
1:A:702:VAL:HG23	1:A:714:ARG:HG3	1.98	0.46
1:A:679:ASN:HD22	1:A:679:ASN:N	2.13	0.46
1:A:238:ARG:O	1:A:263:LEU:HD12	2.16	0.46
1:A:773:ASP:O	1:A:776:PRO:HD2	2.16	0.46
1:A:118:TYR:CE1	1:A:123:LEU:HD13	2.51	0.45
1:A:170:ARG:O	1:A:448:TYR:HE1	1.99	0.45
1:A:202:ARG:O	1:A:204:GLN:N	2.47	0.45
1:A:667:LEU:HD11	1:A:672:VAL:HG21	1.97	0.45
1:A:708:LEU:HD11	1:A:758:ARG:HB2	1.98	0.45
1:A:580:GLU:OE2	1:A:582:GLN:HB2	2.16	0.45
1:A:732:ILE:O	1:A:733:ASP:C	2.58	0.45
1:A:521:GLN:HA	1:A:522:PRO:HA	1.60	0.45
1:A:495:LEU:HA	1:A:495:LEU:HD12	1.62	0.45
1:A:727:LEU:HB2	1:A:732:ILE:CD1	2.46	0.45
1:A:87:GLY:O	1:A:88:VAL:C	2.60	0.45
1:A:301:PRO:HG2	1:A:302:GLU:OE1	2.16	0.45
1:A:709:ALA:HB3	1:A:712:VAL:HG11	1.97	0.45
1:A:7:ARG:HA	1:A:12:HIS:CG	2.52	0.45
1:A:26:LYS:NZ	5:A:2036:HOH:O	2.49	0.45
1:A:458:PHE:CE1	1:A:460:ILE:HD11	2.50	0.45
1:A:773:ASP:HB2	1:A:775:ILE:HG22	1.98	0.45
1:A:397:ARG:HG2	1:A:397:ARG:NH1	2.32	0.45
1:A:675:GLN:O	1:A:679:ASN:HB2	2.16	0.44
1:A:115:ILE:O	5:A:2120:HOH:O	2.21	0.44
1:A:207:GLY:O	1:A:211:LEU:HB2	2.17	0.44
1:A:258:ILE:HB	1:A:438:ASN:HD21	1.81	0.44
1:A:762:LEU:N	1:A:762:LEU:HD13	2.33	0.44
1:A:91:MET:CE	1:A:105:ASN:HB3	2.47	0.44
1:A:499:ILE:HD11	1:A:740:GLY:N	2.29	0.44
1:A:343:SER:HB2	1:A:607:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:754:ILE:HG13	5:A:2465:HOH:O	2.18	0.44
1:A:304:PHE:HA	1:A:356:ASN:HD21	1.83	0.44
1:A:212:GLU:OE2	1:A:212:GLU:N	2.46	0.44
1:A:643:ALA:O	1:A:647:THR:HG23	2.17	0.44
1:A:671:VAL:O	1:A:675:GLN:HG3	2.17	0.44
1:A:765:ASN:N	1:A:767:PRO:HD3	2.33	0.44
1:A:283:GLN:HG2	1:A:320:ASP:O	2.18	0.44
1:A:468:GLN:NE2	1:A:468:GLN:H	2.16	0.43
1:A:745:PHE:N	1:A:745:PHE:CD2	2.86	0.43
1:A:207:GLY:O	1:A:211:LEU:CB	2.67	0.43
1:A:234:ASN:ND2	5:A:2201:HOH:O	2.50	0.43
1:A:562:ARG:NH1	5:A:2373:HOH:O	2.50	0.43
1:A:150:GLU:H	1:A:150:GLU:HG2	1.39	0.43
1:A:246:GLN:CG	1:A:446:LYS:HD2	2.47	0.43
1:A:393:LEU:O	1:A:409:LEU:HD12	2.18	0.43
1:A:600:PHE:O	1:A:603:SER:HB3	2.19	0.43
1:A:391:LYS:HD2	1:A:391:LYS:HA	1.72	0.43
1:A:336:PHE:CE2	1:A:433:LEU:HD23	2.54	0.43
1:A:773:ASP:O	1:A:776:PRO:CD	2.67	0.43
1:A:56:THR:HG23	1:A:59:SER:OG	2.19	0.43
1:A:402:ARG:HG2	1:A:402:ARG:NH1	2.33	0.43
1:A:640:SER:O	1:A:643:ALA:HB3	2.19	0.43
1:A:705:TYR:OH	1:A:755:GLU:HA	2.18	0.43
1:A:728:LYS:O	1:A:731:ASN:N	2.48	0.43
1:A:741:ILE:CG2	1:A:742:THR:HG22	2.46	0.43
1:A:6:ASP:C	1:A:8:THR:H	2.27	0.43
1:A:262:LEU:HD12	1:A:634:TYR:CG	2.54	0.43
1:A:296:LEU:HB2	1:A:298:LEU:HG	2.00	0.43
1:A:149:ASN:OD1	1:A:149:ASN:N	2.40	0.42
1:A:750:GLN:HG2	1:A:754:ILE:CD1	2.49	0.42
1:A:284:LEU:HD13	1:A:345:PHE:HB3	2.00	0.42
1:A:431:LEU:HD22	4:A:1780:PBQ:BR18	2.74	0.42
1:A:732:ILE:HD12	1:A:754:ILE:CD1	2.49	0.42
1:A:171:GLN:NE2	1:A:649:ASN:HB2	2.33	0.42
1:A:173:GLN:HE21	1:A:173:GLN:HB3	1.68	0.42
1:A:775:ILE:N	1:A:776:PRO:HD2	2.33	0.42
1:A:305:ASN:HA	1:A:308:ASN:OD1	2.19	0.42
1:A:661:LYS:NZ	1:A:666:LYS:NZ	2.68	0.42
1:A:704:ARG:HB3	5:A:2460:HOH:O	2.18	0.42
1:A:44:ARG:HH11	1:A:99:GLU:CD	2.28	0.42
1:A:267:ARG:HB3	1:A:278:TYR:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ALA:HB2	1:A:410:ASN:C	2.45	0.42
1:A:657:ILE:O	1:A:675:GLN:NE2	2.50	0.42
1:A:431:LEU:HD22	4:A:1780:PBQ:BR17	2.75	0.42
1:A:459:GLU:OE2	1:A:468:GLN:HG3	2.19	0.42
1:A:717:GLU:O	1:A:718:ASP:HB2	2.20	0.42
1:A:56:THR:OG1	1:A:57:SER:N	2.52	0.42
1:A:147:ARG:NH1	1:A:759:GLU:OE2	2.52	0.42
1:A:266:SER:HA	1:A:423:LYS:HD2	2.02	0.42
1:A:258:ILE:N	1:A:438:ASN:OD1	2.47	0.42
1:A:280:ILE:HG23	1:A:281:PHE:N	2.34	0.42
1:A:291:GLU:HB3	5:A:2229:HOH:O	2.20	0.42
1:A:705:TYR:HE2	1:A:758:ARG:HD3	1.85	0.42
1:A:182:GLY:HA2	1:A:233:ASN:ND2	2.35	0.42
1:A:467:GLU:H	1:A:467:GLU:CD	2.27	0.42
1:A:623:LYS:N	1:A:626:ASN:O	2.52	0.42
1:A:713:PRO:HB2	1:A:715:ASP:H	1.85	0.42
1:A:265:LYS:HE2	4:A:1780:PBQ:H11	1.84	0.41
1:A:422:VAL:HG12	1:A:423:LYS:N	2.34	0.41
1:A:495:LEU:HB3	1:A:496:LYS:CE	2.50	0.41
1:A:586:GLU:HB3	5:A:2399:HOH:O	2.19	0.41
1:A:695:ARG:HB2	1:A:743:LYS:CD	2.47	0.41
1:A:697:ILE:HA	1:A:743:LYS:CB	2.50	0.41
1:A:565:LYS:HB2	1:A:565:LYS:HZ2	1.85	0.41
1:A:727:LEU:O	1:A:731:ASN:N	2.53	0.41
1:A:773:ASP:N	1:A:776:PRO:HD2	2.35	0.41
1:A:72:VAL:HG22	1:A:73:LYS:O	2.18	0.41
1:A:210:VAL:HG12	1:A:211:LEU:N	2.35	0.41
1:A:302:GLU:H	1:A:302:GLU:CD	2.28	0.41
1:A:313:VAL:O	1:A:313:VAL:HG12	2.21	0.41
1:A:319:SER:O	1:A:323:GLU:HG2	2.19	0.41
1:A:430:PHE:O	1:A:431:LEU:C	2.63	0.41
1:A:614:ASP:HA	1:A:615:PRO:HD3	1.91	0.41
1:A:752:ALA:O	1:A:755:GLU:N	2.53	0.41
1:A:109:ARG:O	1:A:114:LEU:HB2	2.20	0.41
1:A:497:GLU:OE1	1:A:497:GLU:HA	2.21	0.41
1:A:205:ALA:O	1:A:208:SER:N	2.52	0.41
1:A:289:THR:O	1:A:292:GLU:N	2.54	0.41
1:A:749:GLY:O	1:A:753:ARG:HD2	2.21	0.41
1:A:2:ASN:HA	1:A:3:PRO:HD3	1.84	0.41
1:A:225:PHE:HE2	1:A:348:ILE:HD11	1.84	0.41
1:A:229:LYS:O	1:A:275:GLU:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:GLN:HB3	1:A:324:PHE:HB2	2.03	0.41
1:A:499:ILE:CD1	1:A:740:GLY:H	2.32	0.41
1:A:530:ASP:O	1:A:533:SER:HB2	2.20	0.41
1:A:702:VAL:HG23	1:A:702:VAL:O	2.18	0.41
1:A:755:GLU:O	1:A:759:GLU:N	2.46	0.41
1:A:741:ILE:HG22	1:A:742:THR:CA	2.50	0.41
1:A:775:ILE:CG2	1:A:776:PRO:HD2	2.51	0.41
1:A:727:LEU:HG	1:A:732:ILE:HG12	2.03	0.40
1:A:753:ARG:O	1:A:756:GLU:HG2	2.21	0.40
1:A:467:GLU:O	1:A:471:ILE:HG13	2.21	0.40
1:A:766:GLU:O	1:A:766:GLU:CG	2.69	0.40
1:A:103:PHE:CE2	1:A:669:ASP:HB3	2.57	0.40
1:A:185:LYS:NZ	1:A:457:GLY:HA3	2.36	0.40
1:A:484:HIS:CD2	1:A:488:LYS:HB3	2.57	0.40
1:A:499:ILE:CD1	1:A:740:GLY:N	2.84	0.40
1:A:716:ALA:HB1	1:A:721:LYS:CE	2.50	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	774/788 (98%)	692 (89%)	72 (9%)	10 (1%)	9 31

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	497	GLU
1	A	713	PRO
1	A	709	ALA
1	A	710	PRO
1	A	766	GLU

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Mol	Chain	Res	Type
1	A	287	GLY
1	A	708	LEU
1	A	712	VAL
1	A	716	ALA
1	A	768	PRO

5.3.2 Protein sidechains ⓘ

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	680/691 (98%)	590 (87%)	90 (13%)	4 14

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	18	LYS
1	A	27	LEU
1	A	31	ASP
1	A	35	ILE
1	A	38	ASN
1	A	41	PRO
1	A	42	LYS
1	A	43	GLU
1	A	44	ARG
1	A	56	THR
1	A	65	VAL
1	A	66	ASP
1	A	71	GLN
1	A	72	VAL
1	A	79	GLN
1	A	82	PRO
1	A	83	ILE
1	A	91	MET
1	A	95	SER
1	A	149	ASN

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Mol	Chain	Res	Type
1	A	150	GLU
1	A	151	VAL
1	A	158	ILE
1	A	171	GLN
1	A	189	THR
1	A	191	LYS
1	A	198	SER
1	A	199	VAL
1	A	204	GLN
1	A	210	VAL
1	A	216	LEU
1	A	277	ASN
1	A	284	LEU
1	A	291	GLU
1	A	294	LYS
1	A	329	GLN
1	A	344	ILE
1	A	358	LYS
1	A	368	VAL
1	A	381	VAL
1	A	387	SER
1	A	402	ARG
1	A	444	GLU
1	A	446	LYS
1	A	495	LEU
1	A	496	LYS
1	A	497	GLU
1	A	498	LYS
1	A	499	ILE
1	A	520	ARG
1	A	565	LYS
1	A	576	GLN
1	A	603	SER
1	A	633	GLN
1	A	646	GLU
1	A	666	LYS
1	A	692	PHE
1	A	695	ARG
1	A	696	ILE
1	A	700	ASP
1	A	702	VAL
1	A	704	ARG

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Mol	Chain	Res	Type
1	A	706	TYR
1	A	707	LEU
1	A	708	LEU
1	A	710	PRO
1	A	717	GLU
1	A	719	SER
1	A	720	GLN
1	A	721	LYS
1	A	726	VAL
1	A	727	LEU
1	A	728	LYS
1	A	730	LEU
1	A	742	THR
1	A	753	ARG
1	A	754	ILE
1	A	755	GLU
1	A	756	GLU
1	A	758	ARG
1	A	762	LEU
1	A	764	SER
1	A	766	GLU
1	A	767	PRO
1	A	769	MET
1	A	771	PHE
1	A	773	ASP
1	A	774	ASP
1	A	777	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	137	GLN
1	A	171	GLN
1	A	173	GLN
1	A	194	GLN
1	A	204	GLN
1	A	206	ASN
1	A	213	GLN
1	A	219	ASN
1	A	234	ASN
1	A	271	GLN

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Mol	Chain	Res	Type
1	A	277	ASN
1	A	329	GLN
1	A	356	ASN
1	A	376	ASN
1	A	407	GLN
1	A	408	HIS
1	A	443	GLN
1	A	464	ASN
1	A	468	GLN
1	A	484	HIS
1	A	500	ASN
1	A	616	ASN
1	A	633	GLN
1	A	651	HIS
1	A	679	ASN
1	A	731	ASN

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 oligosaccharides 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
4	PBQ	A	1780	-	17,18,18	0.62	0	22,27,27	0.96	0
2	AD9	A	1778	3	29,33,33	2.83	7 (24%)	42,52,52	1.20	3 (7%)

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	PBQ	A	1780	-	-	0/4/4/4	0/2/2/2
2	AD9	A	1778	3	-	3/16/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1778	AD9	PA-O3A	8.55	1.68	1.59
2	A	1778	AD9	PB-O3A	8.41	1.68	1.59
2	A	1778	AD9	PB-O1B	5.65	1.70	1.50
2	A	1778	AD9	PA-O2A	3.56	1.71	1.55
2	A	1778	AD9	C4-N3	2.39	1.38	1.34
2	A	1778	AD9	O4'-C1'	2.38	1.47	1.42
2	A	1778	AD9	C8-N9	2.01	1.41	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1778	AD9	O3A-PB-O1B	-3.98	98.72	110.70
2	A	1778	AD9	O2B-PB-O3B	3.03	117.60	107.59
2	A	1778	AD9	O2A-PA-O3A	-2.41	100.77	107.27

There are no chirality outliers.

All (3) torsion outliers are listed below:

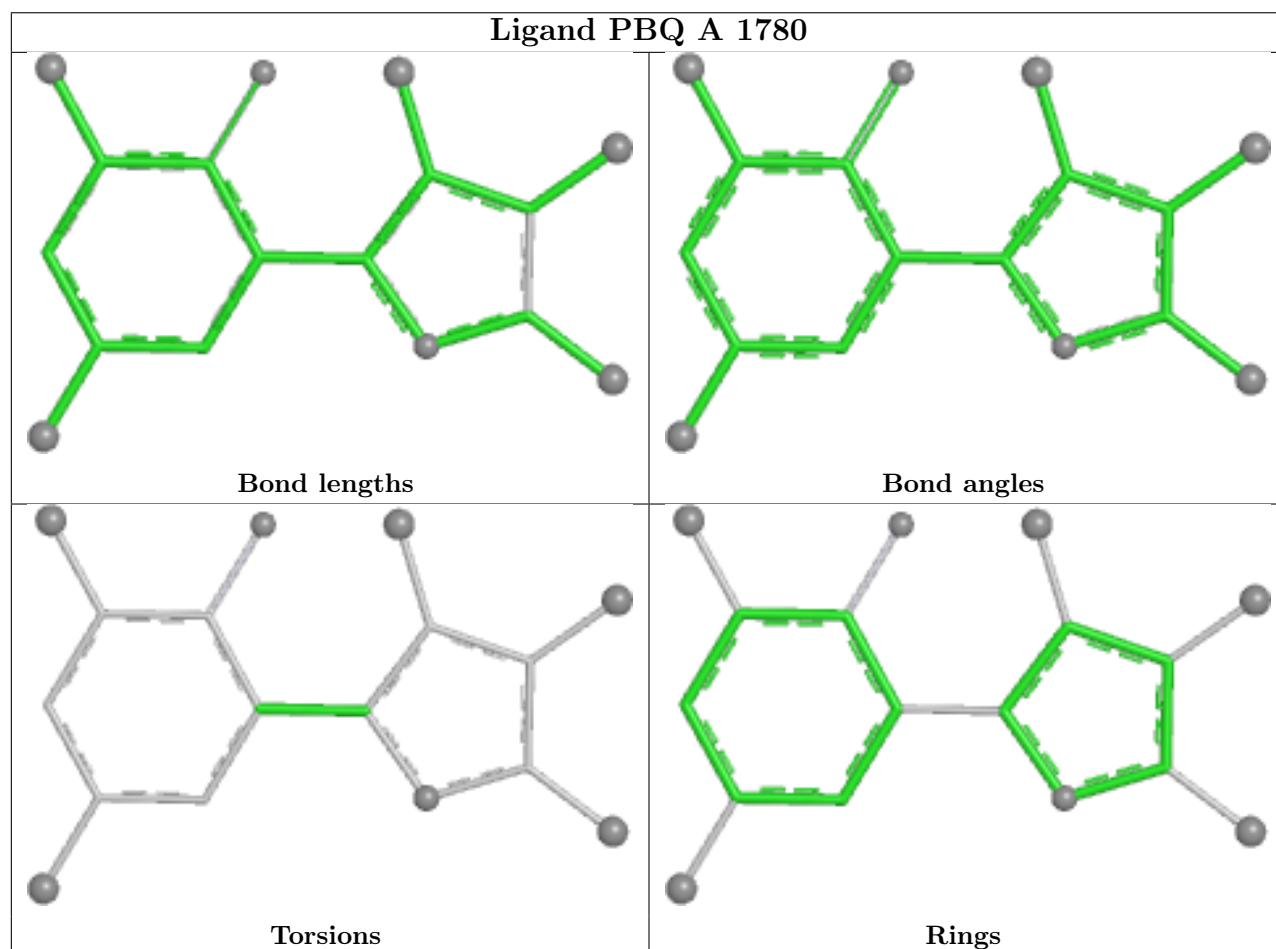
Mol	Chain	Res	Type	Atoms
2	A	1778	AD9	PA-O3A-PB-O1B
2	A	1778	AD9	O4'-C4'-C5'-O5'
2	A	1778	AD9	PA-O3A-PB-O2B

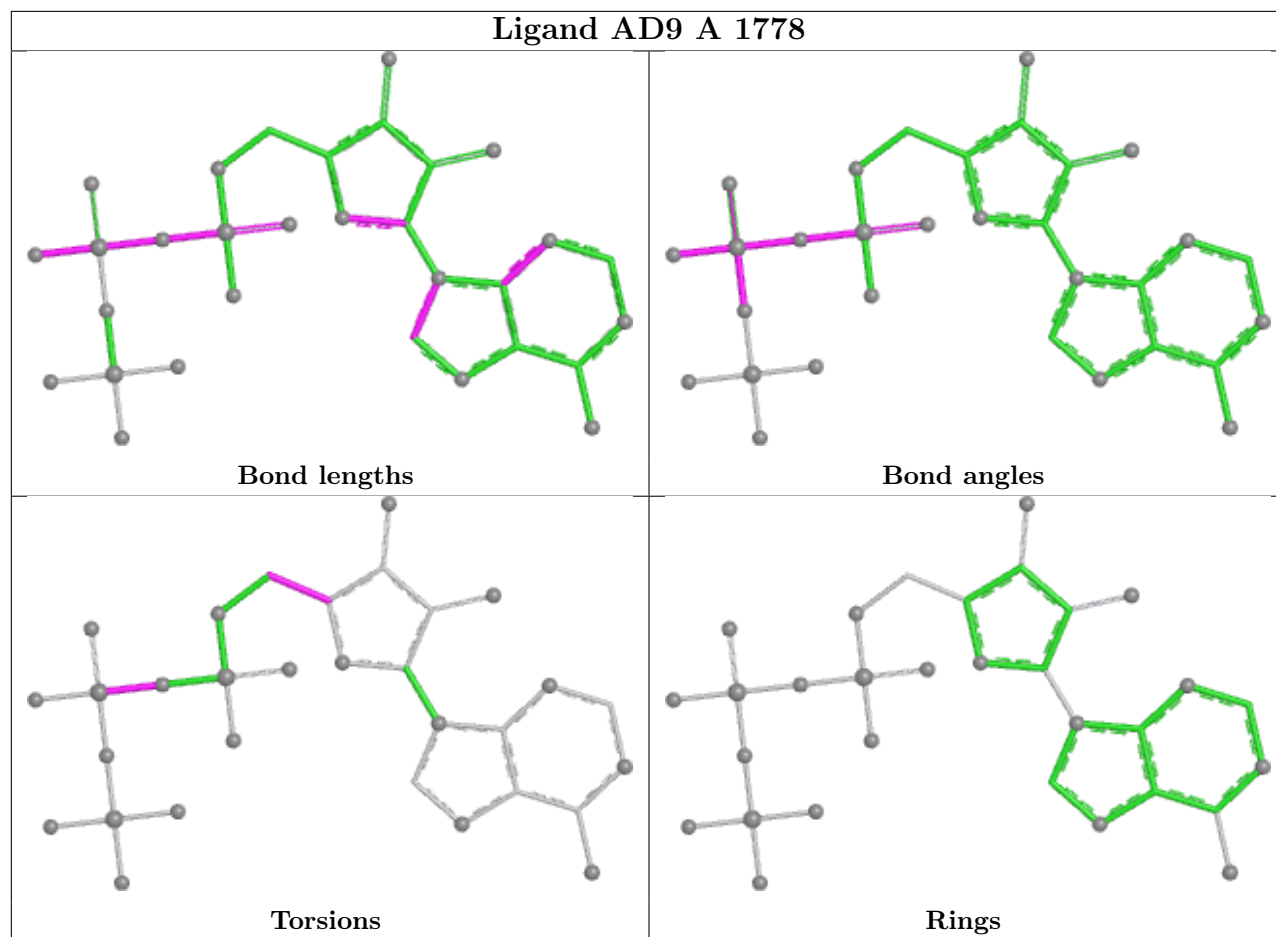
There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1780	PBQ	11	0
2	A	1778	AD9	2	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	747:ARG	C	748:ALA	N	1.16

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, 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	776/788 (98%)	-0.17	42 (5%) 31 24	8, 35, 92, 96	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	208	SER	5.8
1	A	207	GLY	4.7
1	A	708	LEU	3.7
1	A	712	VAL	3.7
1	A	711	ASN	3.6
1	A	209	GLY	3.5
1	A	769	MET	3.5
1	A	736	GLN	3.4
1	A	725	ALA	3.3
1	A	709	ALA	3.3
1	A	765	ASN	3.1
1	A	752	ALA	3.0
1	A	767	PRO	3.0
1	A	206	ASN	3.0
1	A	775	ILE	2.9
1	A	768	PRO	2.9
1	A	755	GLU	2.9
1	A	757	ALA	2.6
1	A	773	ASP	2.6
1	A	719	SER	2.6
1	A	774	ASP	2.6
1	A	742	THR	2.5
1	A	729	HIS	2.5
1	A	762	LEU	2.5
1	A	770	ASP	2.5
1	A	291	GLU	2.4
1	A	727	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	723	THR	2.3
1	A	694	ASN	2.3
1	A	496	LYS	2.3
1	A	750	GLN	2.2
1	A	718	ASP	2.2
1	A	772	ASP	2.2
1	A	702	VAL	2.2
1	A	748	ALA	2.2
1	A	749	GLY	2.1
1	A	699	ALA	2.1
1	A	766	GLU	2.1
1	A	695	ARG	2.1
1	A	722	ALA	2.1
1	A	761	ARG	2.1
1	A	204	GLN	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

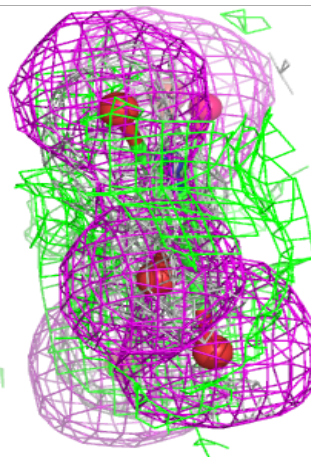
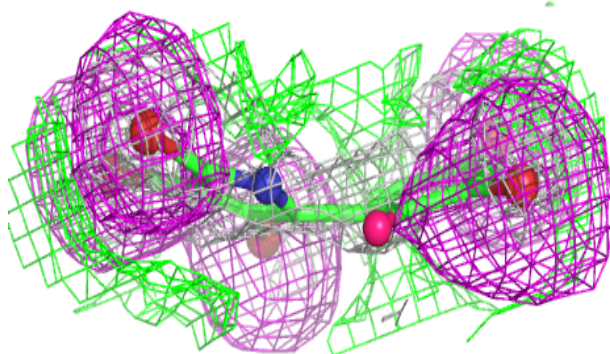
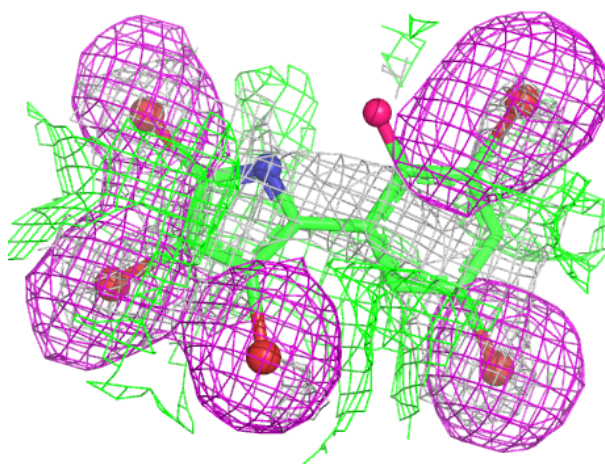
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

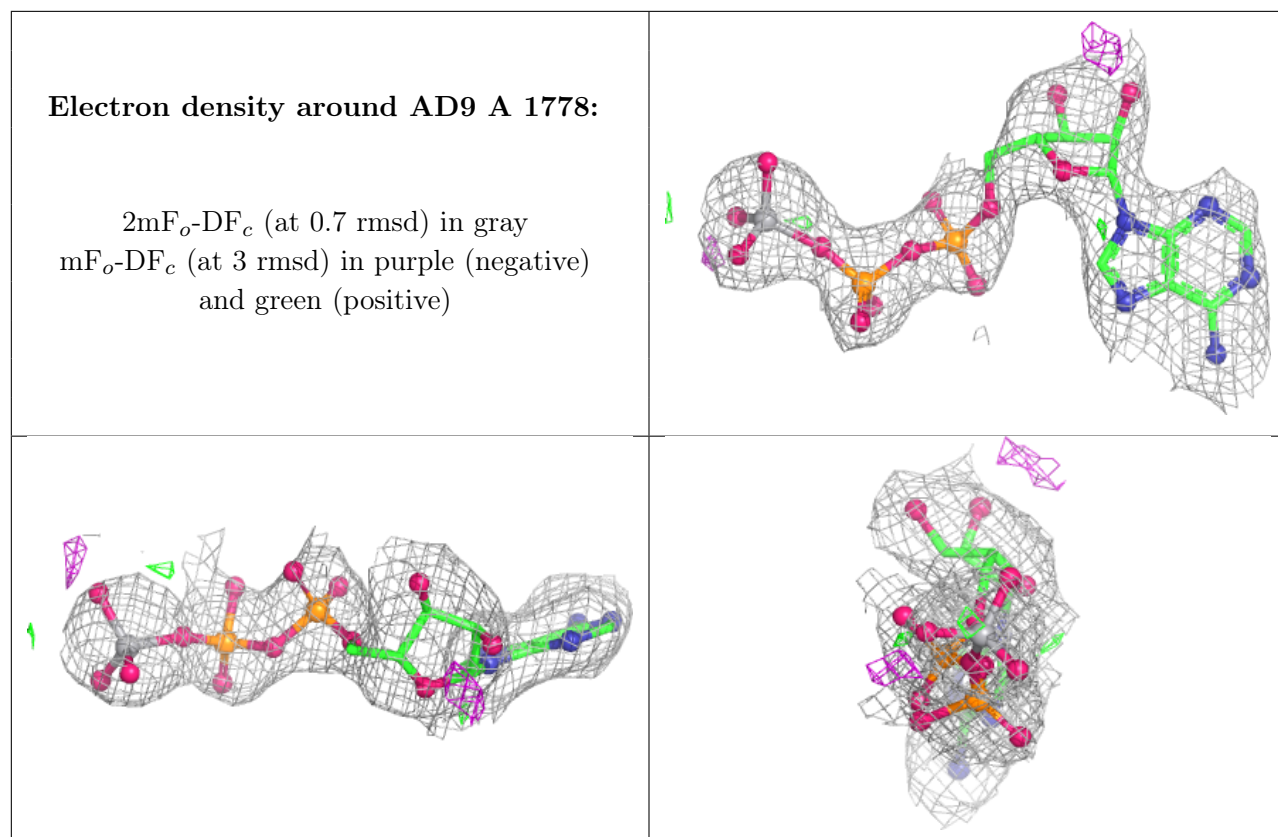
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PBQ	A	1780	17/17	0.51	0.52	31,35,39,41	0
3	MG	A	1779	1/1	0.95	0.12	31,31,31,31	0
2	AD9	A	1778	31/31	0.97	0.07	13,28,36,40	0

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 PBQ A 1780:

$2mF_o-DF_c$ (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.