



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:49 PM UTC

PDB ID : 1S5G / pdb_00001s5g
Title : Structure of Scallop myosin S1 reveals a novel nucleotide conformation
Authors : Risal, D.; Gourinath, S.; Himmel, D.M.; Szent-Gyorgyi, A.G.; Cohen, C.
Deposited on : 2004-01-20
Resolution : 3.10 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

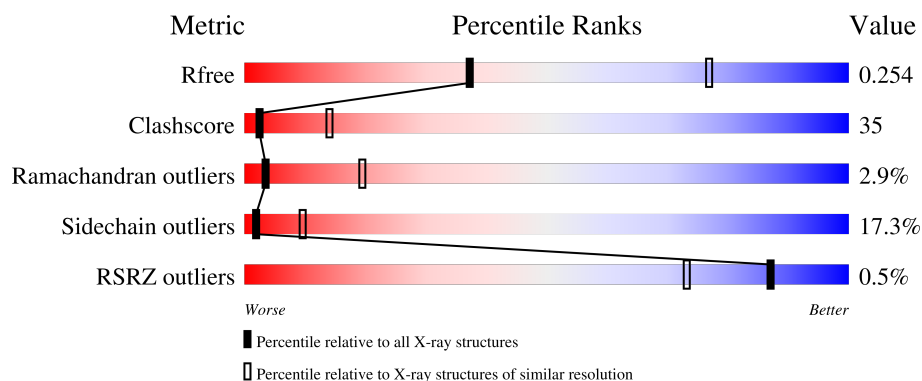
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	840	
2	Y	156	
3	Z	156	

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	SO4	A	996	-	-	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 8607 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 heavy chain, striated muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	802	Total	C	N	O	S	0	0	0
			6301	4020	1075	1168	38			

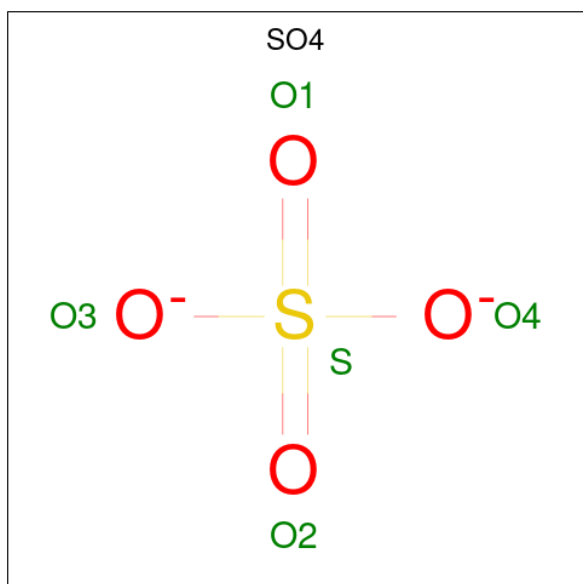
- Molecule 2 is a protein called Myosin regulatory light chain, striated adductor muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	142	Total	C	N	O	S	0	0	0
			1064	665	173	217	9			

- Molecule 3 is a protein called Myosin essential light chain, striated adductor muscle.

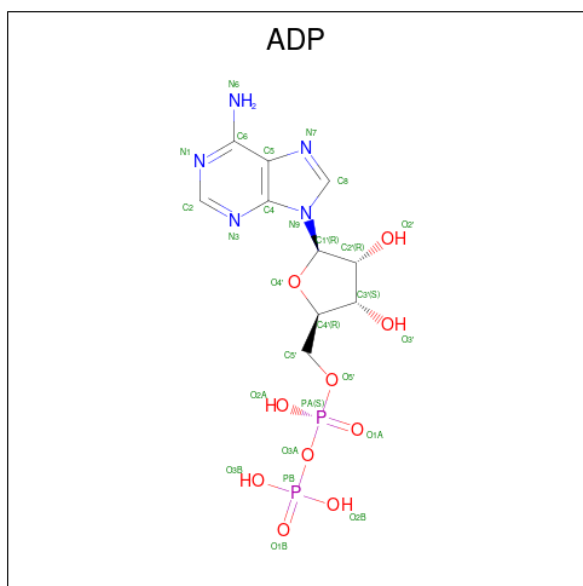
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Z	155	Total	C	N	O	S	0	0	0
			1207	767	190	243	7			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	Y	1	Total	Mg	0	0
			1	1		

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	Z	1	Total	Ca	0	0
			1	1		

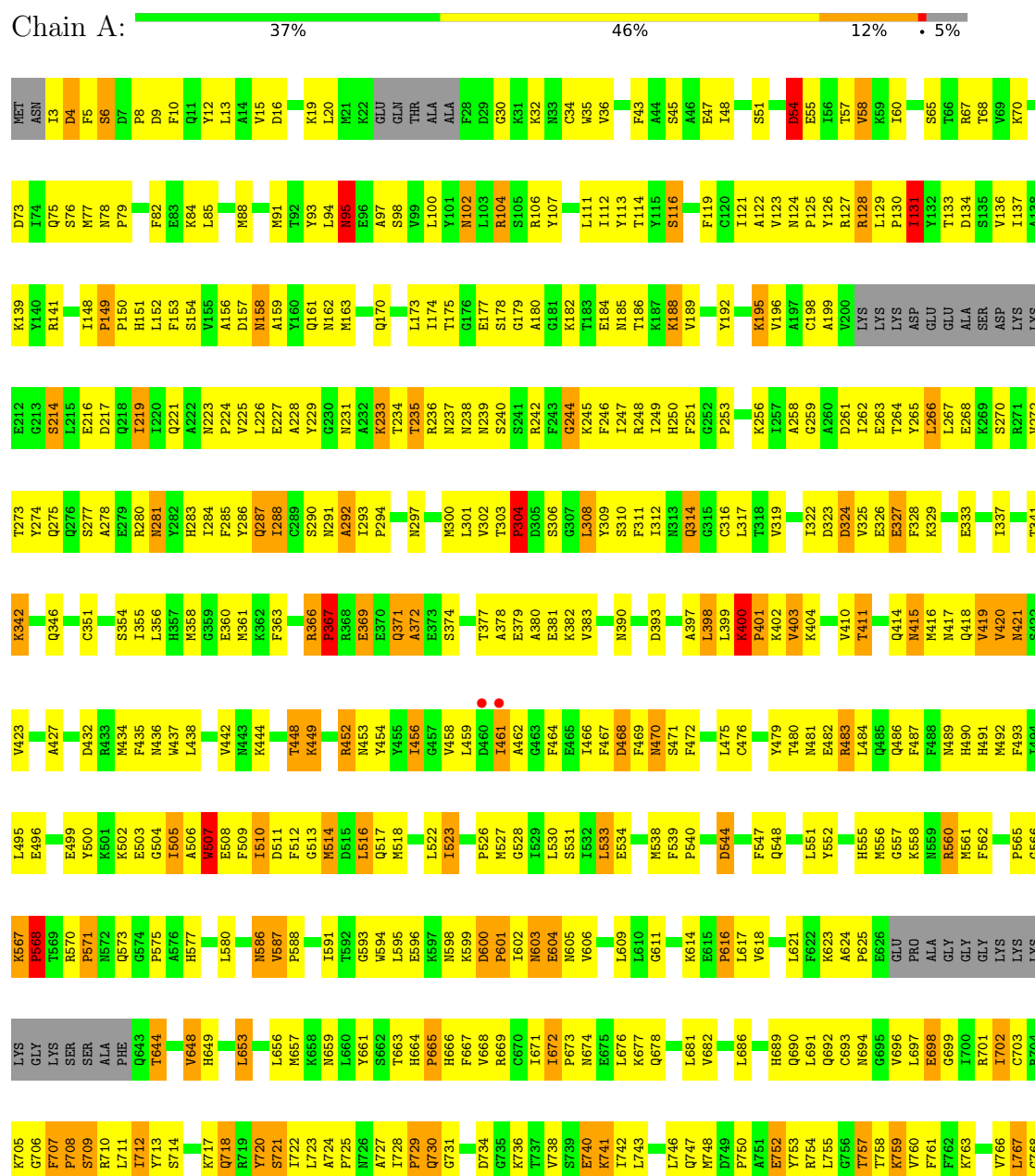
- Molecule 8 is water.

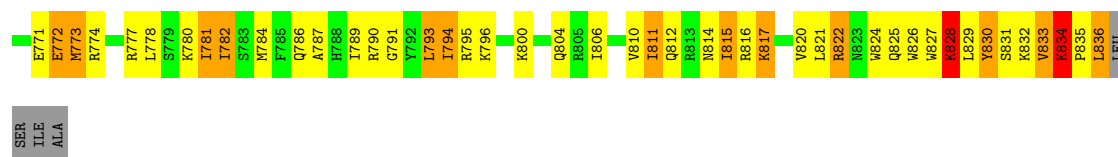
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	O	0	0
			1	1		

3 Residue-property plots

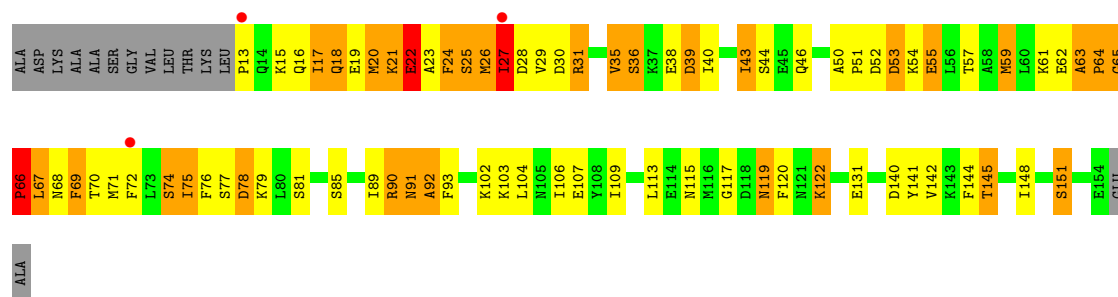
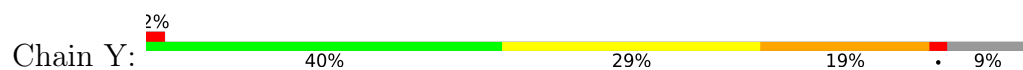
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 heavy chain, striated muscle

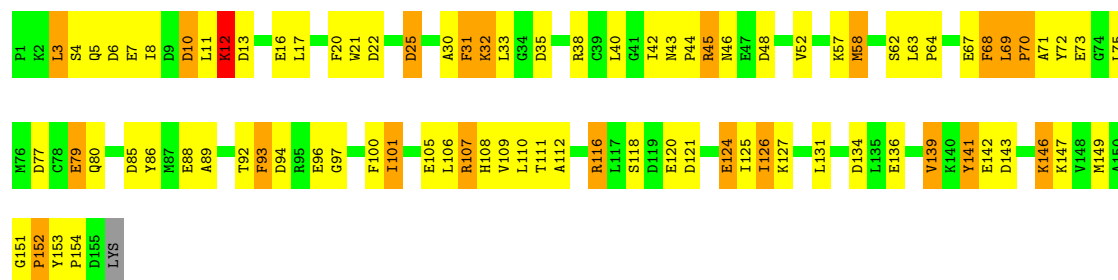




- Molecule 2: Myosin regulatory light chain, striated adductor muscle



- Molecule 3: Myosin essential light chain, striated adductor muscle



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.05Å 50.94Å 161.59Å 90.00° 98.36° 90.00°	Depositor
Resolution (Å)	43.44 – 3.10 43.44 – 3.10	Depositor EDS
% Data completeness (in resolution range)	84.6 (43.44-3.10) 84.6 (43.44-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 3.06Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.233 , 0.269 0.224 , 0.254	Depositor DCC
R_{free} test set	1310 reflections (5.88%)	wwPDB-VP
Wilson B-factor (Å ²)	79.7	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 82.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8607	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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: CA, SO4, ADP, MG

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	0.36	0/6431	1.10	62/8689 (0.7%)
2	Y	0.37	0/1079	1.41	27/1448 (1.9%)
3	Z	0.34	0/1232	1.04	12/1661 (0.7%)
All	All	0.36	0/8742	1.13	101/11798 (0.9%)

There are no bond length outliers.

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	24	PHE	N-CA-C	-10.87	100.75	114.56
2	Y	27	ILE	N-CA-C	-10.21	100.61	110.42
1	A	566	GLY	N-CA-C	-10.14	95.17	112.51
2	Y	55	GLU	N-CA-C	-10.13	100.45	112.92
1	A	624	ALA	CA-C-N	9.66	131.92	119.84
1	A	624	ALA	C-N-CA	9.66	131.92	119.84
1	A	834	LYS	N-CA-C	9.03	129.77	109.81
1	A	54	ASP	N-CA-C	-8.70	102.03	114.12
2	Y	20	MET	N-CA-C	-8.40	103.02	113.18
1	A	539	PHE	CA-C-N	7.79	129.57	119.84
1	A	539	PHE	C-N-CA	7.79	129.57	119.84
2	Y	72	PHE	N-CA-C	-7.67	102.56	112.23
1	A	604	GLU	N-CA-C	-7.67	103.67	112.87
2	Y	65	GLY	N-CA-C	-7.63	96.78	112.34
3	Z	63	LEU	N-CA-C	7.53	123.00	108.85
2	Y	75	ILE	N-CA-C	-7.48	105.06	112.17
2	Y	54	LYS	N-CA-C	-7.42	104.23	113.20
2	Y	18	GLN	N-CA-C	-7.32	103.31	112.90
1	A	523	ILE	N-CA-C	7.31	118.61	111.67
1	A	567	LYS	CA-C-N	7.28	128.94	119.84
1	A	567	LYS	C-N-CA	7.28	128.94	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Y	63	ALA	N-CA-C	7.27	121.74	108.94
1	A	730	GLN	N-CA-C	7.25	122.06	107.41
1	A	834	LYS	CA-C-N	-7.20	111.48	118.97
1	A	834	LYS	C-N-CA	-7.20	111.48	118.97
1	A	219	ILE	N-CA-C	-7.12	102.19	111.09
1	A	755	LEU	N-CA-C	7.11	119.85	108.41
2	Y	92	ALA	N-CA-C	-6.88	103.86	111.36
2	Y	61	LYS	N-CA-C	6.87	120.63	112.93
2	Y	17	ILE	N-CA-C	-6.84	102.99	112.50
1	A	611	GLY	N-CA-C	-6.82	104.03	112.77
3	Z	12	LYS	N-CA-C	-6.76	103.84	111.07
1	A	372	ALA	N-CA-C	6.74	120.50	110.52
1	A	199	ALA	N-CA-C	6.66	120.62	112.23
3	Z	32	LYS	N-CA-C	-6.66	106.36	114.75
1	A	20	LEU	N-CA-C	-6.61	105.19	113.18
1	A	721	SER	N-CA-C	-6.61	103.57	111.69
1	A	624	ALA	N-CA-C	6.53	117.89	109.72
3	Z	3	LEU	N-CA-C	6.49	120.03	109.59
2	Y	23	ALA	N-CA-C	-6.48	103.91	112.72
1	A	664	HIS	CA-C-N	6.48	127.36	120.11
1	A	664	HIS	C-N-CA	6.48	127.36	120.11
2	Y	39	ASP	N-CA-C	-6.46	104.23	111.28
3	Z	93	PHE	N-CA-C	-6.43	106.02	114.31
2	Y	74	SER	N-CA-C	6.41	120.82	113.19
1	A	366	ARG	N-CA-C	6.38	123.91	109.81
2	Y	22	GLU	N-CA-C	-6.36	104.22	112.23
1	A	369	GLU	N-CA-C	-6.36	101.11	110.52
2	Y	50	ALA	CA-C-N	6.32	126.28	119.78
2	Y	50	ALA	C-N-CA	6.32	126.28	119.78
1	A	303	THR	CA-C-N	6.25	127.65	119.84
1	A	303	THR	C-N-CA	6.25	127.65	119.84
1	A	95	ASN	N-CA-C	6.19	117.28	108.74
1	A	483	ARG	N-CA-C	-6.13	104.51	111.07
1	A	738	VAL	N-CA-C	-6.11	104.55	110.42
2	Y	50	ALA	N-CA-C	6.06	119.26	109.15
2	Y	53	ASP	N-CA-C	-6.01	105.44	112.89
2	Y	15	LYS	N-CA-C	5.96	118.73	111.82
1	A	287	GLN	N-CA-C	-5.95	104.70	111.07
1	A	571	PRO	N-CA-C	5.95	124.72	112.47
1	A	555	HIS	N-CA-C	5.89	121.37	113.72
1	A	653	LEU	N-CA-C	-5.86	104.30	112.45
1	A	707	PHE	CA-C-N	5.84	127.14	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	707	PHE	C-N-CA	5.84	127.14	119.84
3	Z	126	ILE	N-CA-C	-5.84	104.64	111.00
1	A	507	TRP	N-CA-C	5.80	123.16	110.80
1	A	587	VAL	N-CA-C	5.74	114.28	107.73
1	A	568	PRO	N-CA-C	5.72	124.25	112.47
2	Y	78	ASP	N-CA-C	-5.66	106.54	113.50
1	A	310	SER	N-CA-C	5.63	119.85	113.15
1	A	828	LYS	N-CA-C	-5.61	105.16	111.28
1	A	131	ILE	CB-CA-C	-5.61	103.74	111.65
3	Z	141	TYR	N-CA-C	5.57	118.12	111.71
1	A	149	PRO	N-CA-C	5.54	117.47	110.70
1	A	342	LYS	N-CA-C	-5.54	105.32	111.36
1	A	570	ARG	CA-C-N	5.54	126.77	119.84
1	A	570	ARG	C-N-CA	5.54	126.77	119.84
1	A	58	VAL	N-CA-C	5.54	115.28	108.53
3	Z	22	ASP	N-CA-C	-5.48	104.85	112.03
2	Y	21	LYS	N-CA-C	-5.36	105.88	112.90
1	A	666	HIS	N-CA-C	-5.35	99.41	110.80
1	A	468	ASP	N-CA-C	-5.33	105.63	111.82
2	Y	115	ASN	N-CA-C	5.32	119.74	112.88
3	Z	151	GLY	CA-C-N	5.31	125.37	119.32
3	Z	151	GLY	C-N-CA	5.31	125.37	119.32
2	Y	151	SER	N-CA-C	-5.30	106.65	113.23
1	A	757	THR	N-CA-C	-5.26	107.24	113.97
1	A	244	GLY	N-CA-C	-5.24	105.03	112.37
1	A	124	ASN	CA-C-N	5.21	124.53	118.85
1	A	124	ASN	C-N-CA	5.21	124.53	118.85
1	A	817	LYS	N-CA-C	-5.21	105.52	111.14
1	A	400	LYS	CA-C-N	5.11	126.23	119.84
1	A	400	LYS	C-N-CA	5.11	126.23	119.84
1	A	292	ALA	N-CA-C	-5.10	106.91	113.23
1	A	698	GLU	N-CA-C	-5.08	105.44	111.69
1	A	281	ASN	N-CA-C	-5.08	102.50	110.17
3	Z	153	TYR	CA-C-N	5.08	126.19	119.84
3	Z	153	TYR	C-N-CA	5.08	126.19	119.84
2	Y	91	ASN	N-CA-C	-5.07	107.76	114.04
1	A	419	VAL	N-CA-C	5.05	115.17	110.42
1	A	720	TYR	N-CA-C	5.04	118.91	112.26

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	6301	0	6170	464	0
2	Y	1064	0	990	76	0
3	Z	1207	0	1127	79	0
4	A	5	0	0	3	0
5	A	27	0	12	5	0
6	Y	1	0	0	0	0
7	Z	1	0	0	0	0
8	A	1	0	0	0	0
All	All	8607	0	8299	587	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 35.

All (587) 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:128:ARG:HH11	1:A:128:ARG:HG3	0.95	1.08
1:A:148:ILE:HG13	1:A:149:PRO:HD2	1.36	1.08
2:Y:35:VAL:HG13	2:Y:39:ASP:HB3	1.33	1.05
2:Y:55:GLU:HA	2:Y:59:MET:HE3	1.42	0.99
1:A:128:ARG:HG3	1:A:128:ARG:NH1	1.75	0.96
1:A:507:TRP:CG	1:A:508:GLU:H	1.83	0.94
1:A:822:ARG:CB	1:A:822:ARG:HH11	1.81	0.92
1:A:468:ASP:HB3	1:A:573:GLN:HA	1.53	0.91
1:A:723:LEU:HD23	1:A:746:LEU:HD11	1.51	0.91
3:Z:52:VAL:HG21	3:Z:75:LEU:HD21	1.51	0.89
1:A:253:PRO:HG3	1:A:453:ASN:ND2	1.89	0.87
1:A:48:ILE:HA	1:A:58:VAL:HG12	1.56	0.87
1:A:319:VAL:HB	1:A:322:ILE:HB	1.57	0.87
3:Z:5:GLN:HA	3:Z:8:ILE:HD12	1.57	0.86
1:A:448:THR:H	1:A:452:ARG:HH22	1.21	0.86
1:A:523:ILE:HD11	1:A:580:LEU:HD21	1.58	0.86
1:A:128:ARG:HH11	1:A:128:ARG:CG	1.86	0.85
1:A:292:ALA:HB2	1:A:325:VAL:HG13	1.59	0.84
1:A:796:LYS:HD3	3:Z:152:PRO:HB3	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:69:LEU:HB3	3:Z:70:PRO:HD3	1.59	0.84
1:A:361:MET:HE2	1:A:380:ALA:HA	1.60	0.83
1:A:483:ARG:HB3	1:A:657:MET:HE2	1.60	0.83
1:A:55:GLU:HG3	1:A:68:THR:HG21	1.60	0.83
1:A:291:ASN:HD22	1:A:304:PRO:HG2	1.44	0.82
1:A:290:SER:HB2	1:A:325:VAL:HG22	1.61	0.82
1:A:239:ASN:HB3	5:A:995:ADP:O2A	1.79	0.81
1:A:717:LYS:HG3	1:A:718:GLN:N	1.95	0.80
1:A:401:PRO:HG3	1:A:603:ASN:HD21	1.46	0.80
1:A:522:LEU:HD11	1:A:562:PHE:HB2	1.64	0.80
1:A:470:ASN:N	1:A:470:ASN:HD22	1.79	0.80
1:A:603:ASN:HB3	1:A:606:VAL:H	1.47	0.79
1:A:180:ALA:HA	1:A:672:ILE:HG23	1.64	0.79
1:A:567:LYS:HB3	1:A:568:PRO:HD2	1.64	0.79
1:A:148:ILE:HG13	1:A:149:PRO:CD	2.12	0.79
1:A:836:LEU:HD22	2:Y:26:MET:SD	2.23	0.78
1:A:182:LYS:HG2	4:A:996:SO4:O2	1.83	0.78
1:A:780:LYS:HG2	1:A:784:MET:HE3	1.65	0.78
1:A:822:ARG:HH11	1:A:822:ARG:HB2	1.48	0.78
1:A:157:ASP:HB2	1:A:192:TYR:OH	1.85	0.77
1:A:829:LEU:O	1:A:833:VAL:HG23	1.85	0.76
1:A:186:THR:HG23	1:A:458:VAL:HG11	1.67	0.75
1:A:123:VAL:HG12	1:A:673:PRO:HG3	1.68	0.75
1:A:509:PHE:O	1:A:510:ILE:HG23	1.87	0.75
2:Y:21:LYS:O	2:Y:24:PHE:HB3	1.87	0.74
1:A:796:LYS:CD	3:Z:152:PRO:HB3	2.18	0.74
1:A:107:TYR:HA	1:A:111:LEU:O	1.86	0.74
1:A:55:GLU:HG3	1:A:68:THR:CG2	2.19	0.73
1:A:507:TRP:CG	1:A:508:GLU:N	2.49	0.73
1:A:507:TRP:CD1	1:A:508:GLU:H	2.06	0.73
1:A:834:LYS:HA	1:A:836:LEU:HD23	1.69	0.73
1:A:287:GLN:HB3	1:A:328:PHE:HB2	1.70	0.73
1:A:227:GLU:HA	1:A:231:ASN:OD1	1.88	0.72
1:A:707:PHE:CE1	1:A:754:ARG:HD2	2.23	0.72
3:Z:42:ILE:HG22	3:Z:44:PRO:HD3	1.71	0.72
1:A:112:ILE:HD13	1:A:125:PRO:HG3	1.71	0.71
2:Y:40:ILE:O	2:Y:43:ILE:HG23	1.90	0.71
1:A:833:VAL:HG12	1:A:833:VAL:O	1.90	0.71
1:A:459:LEU:HD11	1:A:461:ILE:HD11	1.73	0.70
1:A:603:ASN:HD22	1:A:605:ASN:HB3	1.56	0.70
1:A:13:LEU:HD21	1:A:131:ILE:CG2	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:42:ILE:C	3:Z:44:PRO:HD3	2.17	0.70
1:A:727:ALA:O	1:A:729:PRO:HD3	1.91	0.70
1:A:448:THR:H	1:A:452:ARG:NH2	1.90	0.70
1:A:70:LYS:O	1:A:73:ASP:HB2	1.91	0.70
1:A:414:GLN:HB2	1:A:418:GLN:HB2	1.74	0.69
1:A:672:ILE:H	1:A:672:ILE:HD13	1.56	0.69
3:Z:31:PHE:CD2	3:Z:58:MET:HG2	2.27	0.69
1:A:694:ASN:HD22	1:A:696:VAL:HG13	1.57	0.69
1:A:292:ALA:C	1:A:293:ILE:HD12	2.18	0.69
1:A:378:ALA:O	1:A:382:LYS:HG3	1.93	0.69
1:A:784:MET:HE1	3:Z:79:GLU:OE1	1.93	0.69
1:A:128:ARG:HA	5:A:995:ADP:H2	1.57	0.68
1:A:758:THR:HG23	1:A:759:LYS:HD3	1.75	0.68
1:A:707:PHE:HB3	1:A:761:PHE:HB3	1.74	0.68
2:Y:63:ALA:O	2:Y:65:GLY:N	2.24	0.68
3:Z:69:LEU:O	3:Z:73:GLU:HG2	1.94	0.68
1:A:221:GLN:O	1:A:224:PRO:HD2	1.93	0.68
1:A:244:GLY:HA3	1:A:461:ILE:HG23	1.76	0.68
1:A:377:THR:O	1:A:381:GLU:HG3	1.94	0.68
1:A:291:ASN:HB2	1:A:304:PRO:HB3	1.74	0.67
1:A:746:LEU:CD2	1:A:773:MET:HE1	2.23	0.67
1:A:469:PHE:C	1:A:470:ASN:HD22	2.01	0.67
1:A:363:PHE:HD2	1:A:374:SER:HA	1.60	0.67
1:A:694:ASN:ND2	1:A:696:VAL:HG13	2.10	0.67
1:A:280:ARG:HG2	1:A:316:CYS:O	1.95	0.67
1:A:800:LYS:O	1:A:804:GLN:HG3	1.95	0.66
1:A:468:ASP:CB	1:A:573:GLN:HA	2.25	0.66
1:A:812:GLN:O	1:A:816:ARG:HG3	1.95	0.66
1:A:106:ARG:HG2	1:A:111:LEU:HD12	1.77	0.66
1:A:834:LYS:O	1:A:834:LYS:HD3	1.96	0.66
1:A:822:ARG:HH11	1:A:822:ARG:CG	2.08	0.66
2:Y:18:GLN:O	2:Y:21:LYS:HB3	1.96	0.66
1:A:717:LYS:HG3	1:A:718:GLN:H	1.61	0.65
1:A:229:TYR:CZ	1:A:284:ILE:HG12	2.30	0.65
2:Y:27:ILE:HG22	2:Y:28:ASP:N	2.11	0.65
2:Y:35:VAL:CG1	2:Y:40:ILE:HG13	2.26	0.65
3:Z:71:ALA:O	3:Z:75:LEU:HD23	1.97	0.65
1:A:342:LYS:O	1:A:346:GLN:HG3	1.96	0.65
1:A:522:LEU:HD12	1:A:561:MET:HB2	1.78	0.65
1:A:711:LEU:O	1:A:759:LYS:HB2	1.97	0.65
1:A:830:TYR:HD2	1:A:830:TYR:C	2.05	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:70:THR:HG22	2:Y:70:THR:O	1.98	0.64
1:A:398:LEU:HD21	1:A:423:VAL:HG22	1.79	0.64
1:A:13:LEU:HD21	1:A:131:ILE:HG21	1.78	0.64
1:A:789:ILE:HG23	3:Z:125:ILE:HD12	1.80	0.64
1:A:123:VAL:CG1	1:A:673:PRO:HG3	2.28	0.64
1:A:586:ASN:N	1:A:586:ASN:HD22	1.95	0.64
1:A:470:ASN:N	1:A:470:ASN:ND2	2.39	0.63
1:A:399:LEU:C	1:A:401:PRO:HD3	2.23	0.63
2:Y:75:ILE:O	2:Y:75:ILE:HG22	1.98	0.63
2:Y:35:VAL:HG13	2:Y:39:ASP:CB	2.20	0.63
3:Z:31:PHE:HD2	3:Z:58:MET:HG2	1.61	0.63
1:A:79:PRO:HD2	1:A:82:PHE:CD1	2.33	0.63
1:A:354:SER:O	1:A:358:MET:HG3	1.98	0.63
1:A:686:LEU:O	1:A:690:GLN:HG3	1.98	0.63
1:A:690:GLN:O	1:A:694:ASN:N	2.32	0.63
1:A:267:LEU:HD12	1:A:268:GLU:H	1.62	0.63
1:A:746:LEU:HD21	1:A:773:MET:HE1	1.80	0.62
2:Y:27:ILE:HG23	2:Y:35:VAL:HG21	1.82	0.62
1:A:5:PHE:CG	1:A:6:SER:N	2.62	0.62
1:A:568:PRO:HA	1:A:573:GLN:OE1	2.00	0.62
2:Y:35:VAL:CG1	2:Y:39:ASP:HB3	2.22	0.62
1:A:170:GLN:O	1:A:456:ILE:HA	1.99	0.61
1:A:691:LEU:HD22	1:A:696:VAL:HG21	1.81	0.61
1:A:154:SER:O	1:A:158:ASN:HB2	2.00	0.61
1:A:781:ILE:HG21	3:Z:85:ASP:O	2.01	0.61
1:A:128:ARG:HD2	1:A:128:ARG:N	2.16	0.61
3:Z:142:GLU:O	3:Z:146:LYS:HG2	2.01	0.61
1:A:286:TYR:HE2	1:A:317:LEU:HD23	1.64	0.61
1:A:371:GLN:HG3	1:A:372:ALA:N	2.15	0.61
1:A:410:VAL:HG12	1:A:411:THR:N	2.16	0.61
1:A:577:HIS:ND1	1:A:591:ILE:HG12	2.14	0.61
1:A:690:GLN:O	1:A:694:ASN:HB2	2.01	0.61
1:A:248:ARG:C	1:A:249:ILE:HD12	2.26	0.61
1:A:479:TYR:O	1:A:482:GLU:HB3	2.01	0.61
1:A:676:LEU:HD12	1:A:681:LEU:CD2	2.31	0.61
1:A:826:TRP:HZ2	2:Y:59:MET:SD	2.24	0.61
1:A:830:TYR:C	1:A:830:TYR:CD2	2.77	0.60
1:A:186:THR:HG23	1:A:458:VAL:CG1	2.31	0.60
1:A:119:PHE:CE1	1:A:696:VAL:HA	2.36	0.60
1:A:113:TYR:O	1:A:150:PRO:HB2	2.02	0.60
3:Z:111:THR:O	3:Z:116:ARG:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:781:ILE:HG21	3:Z:89:ALA:HB2	1.83	0.60
1:A:292:ALA:CB	1:A:325:VAL:HG13	2.29	0.60
2:Y:24:PHE:CG	2:Y:69:PHE:HB2	2.37	0.60
1:A:264:THR:HG21	1:A:435:PHE:HE1	1.66	0.59
1:A:351:CYS:SG	1:A:617:LEU:HD23	2.41	0.59
2:Y:122:LYS:H	2:Y:122:LYS:HD2	1.67	0.59
1:A:698:GLU:O	1:A:702:ILE:HG23	2.03	0.59
1:A:133:THR:O	1:A:137:ILE:HG13	2.03	0.59
1:A:288:ILE:HD12	1:A:300:MET:SD	2.43	0.58
1:A:522:LEU:HD13	1:A:580:LEU:HD11	1.85	0.58
1:A:486:GLN:HE22	1:A:517:GLN:HG2	1.67	0.58
1:A:728:ILE:O	1:A:729:PRO:C	2.46	0.58
1:A:88:MET:HA	1:A:91:MET:HG3	1.85	0.58
1:A:533:LEU:HD11	1:A:594:TRP:HB3	1.85	0.58
1:A:244:GLY:CA	1:A:461:ILE:HG23	2.33	0.58
1:A:170:GLN:HB2	1:A:456:ILE:HB	1.86	0.58
1:A:239:ASN:CB	5:A:995:ADP:O2A	2.49	0.58
1:A:674:ASN:ND2	1:A:681:LEU:HB3	2.18	0.58
2:Y:122:LYS:HD2	2:Y:122:LYS:N	2.18	0.58
1:A:696:VAL:HG23	1:A:697:LEU:H	1.67	0.58
1:A:499:GLU:HG2	1:A:710:ARG:NH1	2.19	0.58
3:Z:69:LEU:HB3	3:Z:70:PRO:CD	2.31	0.58
1:A:180:ALA:CA	1:A:672:ILE:HG23	2.33	0.57
1:A:791:GLY:O	1:A:795:ARG:HB2	2.03	0.57
1:A:741:LYS:HD3	1:A:741:LYS:C	2.29	0.57
2:Y:55:GLU:CA	2:Y:59:MET:HE3	2.25	0.57
2:Y:144:PHE:O	2:Y:148:ILE:HG12	2.04	0.57
1:A:192:TYR:O	1:A:196:VAL:HG22	2.04	0.57
1:A:262:ILE:HG22	1:A:263:GLU:N	2.19	0.57
1:A:156:ALA:O	1:A:159:ALA:HB3	2.05	0.57
1:A:297:ASN:N	1:A:297:ASN:HD22	2.02	0.57
1:A:489:ASN:HB3	1:A:512:PHE:CB	2.35	0.57
1:A:511:ASP:OD1	1:A:513:GLY:N	2.36	0.57
1:A:267:LEU:HD12	1:A:268:GLU:N	2.18	0.57
1:A:603:ASN:C	1:A:605:ASN:N	2.58	0.57
1:A:112:ILE:O	1:A:122:ALA:HA	2.04	0.57
1:A:397:ALA:O	1:A:401:PRO:HG3	2.04	0.57
1:A:174:ILE:HD13	1:A:668:VAL:HB	1.86	0.57
1:A:240:SER:OG	1:A:242:ARG:HD3	2.05	0.57
1:A:724:ALA:N	1:A:725:PRO:HD3	2.20	0.57
1:A:830:TYR:HD1	2:Y:76:PHE:HE2	1.53	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:105:GLU:O	3:Z:108:HIS:HB3	2.05	0.57
1:A:272:VAL:HA	1:A:281:ASN:HD21	1.70	0.56
1:A:60:ILE:HD12	1:A:60:ILE:N	2.20	0.56
1:A:128:ARG:HD2	1:A:128:ARG:H	1.71	0.56
1:A:184:GLU:O	1:A:188:LYS:HD2	2.05	0.56
1:A:264:THR:HG21	1:A:435:PHE:CE1	2.41	0.56
1:A:456:ILE:O	1:A:456:ILE:HG13	2.05	0.56
1:A:523:ILE:HD11	1:A:580:LEU:CD2	2.33	0.56
2:Y:63:ALA:HB1	2:Y:66:PRO:O	2.05	0.56
1:A:151:HIS:ND1	1:A:152:LEU:N	2.53	0.56
1:A:293:ILE:HG22	1:A:293:ILE:O	2.05	0.56
1:A:702:ILE:O	1:A:705:LYS:HG2	2.05	0.56
1:A:742:ILE:O	1:A:746:LEU:HB2	2.05	0.56
3:Z:12:LYS:HD2	3:Z:16:GLU:OE1	2.06	0.56
3:Z:86:TYR:O	3:Z:89:ALA:HB3	2.05	0.56
1:A:214:SER:O	1:A:217:ASP:HB2	2.03	0.56
1:A:249:ILE:HG22	1:A:251:PHE:CE1	2.40	0.56
1:A:741:LYS:HD3	1:A:741:LYS:O	2.05	0.56
1:A:811:ILE:HD11	2:Y:93:PHE:N	2.21	0.56
1:A:830:TYR:HD1	2:Y:76:PHE:CE2	2.24	0.56
1:A:119:PHE:HE1	1:A:696:VAL:HA	1.69	0.56
1:A:475:LEU:HD23	1:A:475:LEU:C	2.30	0.56
1:A:696:VAL:HG23	1:A:697:LEU:N	2.21	0.56
3:Z:30:ALA:C	3:Z:32:LYS:H	2.14	0.56
1:A:390:ASN:HB3	1:A:393:ASP:HB2	1.87	0.55
1:A:728:ILE:HG22	1:A:729:PRO:O	2.06	0.55
1:A:227:GLU:O	1:A:231:ASN:HB2	2.06	0.55
1:A:227:GLU:CD	1:A:239:ASN:HD21	2.14	0.55
1:A:291:ASN:ND2	1:A:304:PRO:HG2	2.18	0.55
1:A:603:ASN:C	1:A:605:ASN:H	2.13	0.55
1:A:753:TYR:O	1:A:754:ARG:HG3	2.07	0.55
3:Z:31:PHE:CG	3:Z:31:PHE:O	2.59	0.55
1:A:221:GLN:C	1:A:224:PRO:HD2	2.32	0.55
1:A:231:ASN:HA	1:A:240:SER:O	2.06	0.55
1:A:593:GLY:O	1:A:596:GLU:HG2	2.07	0.55
1:A:173:LEU:HD12	1:A:173:LEU:N	2.22	0.54
1:A:432:ASP:OD1	1:A:436:ASN:ND2	2.41	0.54
3:Z:10:ASP:O	3:Z:13:ASP:HB2	2.07	0.54
1:A:728:ILE:C	1:A:729:PRO:O	2.48	0.54
2:Y:106:ILE:HG23	2:Y:107:GLU:N	2.23	0.54
2:Y:131:GLU:O	2:Y:131:GLU:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:VAL:HG12	1:A:16:ASP:N	2.23	0.54
1:A:665:PRO:HB3	1:A:667:PHE:CZ	2.42	0.54
3:Z:88:GLU:O	3:Z:92:THR:HG23	2.08	0.54
1:A:806:ILE:O	1:A:810:VAL:HG23	2.07	0.54
3:Z:101:ILE:HG22	3:Z:141:TYR:HD1	1.73	0.54
1:A:79:PRO:HD2	1:A:82:PHE:HD1	1.72	0.54
2:Y:122:LYS:H	2:Y:122:LYS:CD	2.19	0.54
1:A:9:ASP:HB3	1:A:136:VAL:HG22	1.90	0.53
1:A:262:ILE:HG22	1:A:263:GLU:H	1.72	0.53
1:A:198:CYS:O	1:A:256:LYS:HD2	2.09	0.53
1:A:829:LEU:HD21	2:Y:40:ILE:HG23	1.90	0.53
3:Z:120:GLU:O	3:Z:124:GLU:HB2	2.08	0.53
1:A:216:GLU:HA	1:A:219:ILE:HD13	1.91	0.53
1:A:692:GLN:HA	1:A:697:LEU:HD12	1.90	0.53
3:Z:40:LEU:HD12	3:Z:72:TYR:CE1	2.43	0.53
1:A:484:LEU:O	1:A:487:PHE:HB3	2.09	0.53
1:A:614:LYS:O	1:A:616:PRO:HD3	2.08	0.53
1:A:287:GLN:HB3	1:A:328:PHE:CB	2.37	0.53
1:A:599:LYS:O	1:A:601:PRO:HD3	2.08	0.53
1:A:505:ILE:CD1	1:A:754:ARG:HB3	2.38	0.53
1:A:707:PHE:CZ	1:A:754:ARG:HD2	2.44	0.53
2:Y:36:SER:N	2:Y:39:ASP:HB2	2.23	0.53
1:A:128:ARG:HH21	5:A:995:ADP:H2'	1.74	0.53
1:A:275:GLN:NE2	1:A:281:ASN:HD22	2.07	0.53
1:A:499:GLU:O	1:A:502:LYS:HB3	2.09	0.53
1:A:736:LYS:O	1:A:740:GLU:N	2.35	0.53
1:A:834:LYS:HA	1:A:836:LEU:CD2	2.38	0.53
2:Y:22:GLU:O	2:Y:25:SER:HB2	2.09	0.53
1:A:128:ARG:NH2	5:A:995:ADP:H2'	2.24	0.53
1:A:671:ILE:HG23	1:A:690:GLN:CD	2.34	0.52
1:A:491:HIS:NE2	1:A:495:LEU:HD11	2.24	0.52
1:A:707:PHE:HE2	1:A:763:LYS:HG2	1.75	0.52
1:A:518:MET:HB3	1:A:561:MET:HE2	1.90	0.52
1:A:789:ILE:HG12	3:Z:125:ILE:HD13	1.91	0.52
1:A:291:ASN:HB2	1:A:304:PRO:CB	2.40	0.52
1:A:414:GLN:HE21	1:A:419:VAL:HG22	1.74	0.52
1:A:547:PHE:CZ	1:A:551:LEU:HD11	2.44	0.52
1:A:811:ILE:HD11	2:Y:92:ALA:C	2.35	0.52
1:A:261:ASP:C	1:A:261:ASP:OD1	2.53	0.52
1:A:106:ARG:HB3	1:A:111:LEU:HB2	1.90	0.52
2:Y:13:PRO:HB3	2:Y:17:ILE:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:LEU:HD11	1:A:774:ARG:HA	1.91	0.52
2:Y:39:ASP:O	2:Y:43:ILE:HG22	2.10	0.52
3:Z:42:ILE:HG22	3:Z:44:PRO:CD	2.39	0.51
1:A:448:THR:N	1:A:452:ARG:HH22	2.00	0.51
1:A:721:SER:HA	1:A:742:ILE:HD11	1.92	0.51
1:A:195:LYS:O	1:A:195:LYS:HG3	2.09	0.51
1:A:481:ASN:HA	1:A:484:LEU:HB2	1.92	0.51
1:A:707:PHE:CB	1:A:761:PHE:HB3	2.40	0.51
1:A:784:MET:CE	3:Z:79:GLU:HB3	2.41	0.51
1:A:355:ILE:HG22	1:A:355:ILE:O	2.09	0.51
1:A:490:HIS:O	1:A:493:PHE:HB3	2.10	0.51
1:A:185:ASN:O	1:A:189:VAL:HG23	2.10	0.51
1:A:363:PHE:CD2	1:A:374:SER:HA	2.43	0.51
1:A:600:ASP:O	1:A:602:ILE:HG12	2.11	0.51
1:A:259:GLY:HA3	1:A:452:ARG:HH12	1.76	0.51
1:A:467:PHE:C	1:A:470:ASN:HD21	2.19	0.51
2:Y:25:SER:HB3	2:Y:26:MET:HE3	1.92	0.51
1:A:518:MET:HE1	1:A:560:ARG:CZ	2.40	0.51
2:Y:102:LYS:O	2:Y:103:LYS:HG3	2.11	0.51
1:A:134:ASP:O	1:A:137:ILE:HB	2.11	0.51
1:A:591:ILE:HA	1:A:594:TRP:CE2	2.46	0.50
1:A:13:LEU:HD21	1:A:131:ILE:HG23	1.94	0.50
1:A:489:ASN:N	1:A:489:ASN:HD22	2.10	0.50
1:A:500:TYR:HB3	1:A:506:ALA:HA	1.94	0.50
1:A:4:ASP:HB3	1:A:10:PHE:CE2	2.46	0.50
1:A:758:THR:HG23	1:A:759:LYS:CD	2.41	0.50
1:A:100:LEU:HD12	1:A:100:LEU:O	2.12	0.50
1:A:178:SER:O	1:A:236:ARG:HG2	2.12	0.50
1:A:707:PHE:CE2	1:A:763:LYS:HG2	2.47	0.50
3:Z:33:LEU:HA	3:Z:68:PHE:CZ	2.46	0.50
1:A:603:ASN:CB	1:A:606:VAL:HG23	2.42	0.49
2:Y:62:GLU:O	2:Y:75:ILE:HG23	2.12	0.49
3:Z:44:PRO:HB3	3:Z:75:LEU:HD12	1.92	0.49
1:A:489:ASN:HB3	1:A:512:PHE:HB2	1.93	0.49
1:A:618:VAL:HA	1:A:621:LEU:HD12	1.94	0.49
1:A:54:ASP:O	1:A:70:LYS:HA	2.13	0.49
1:A:78:ASN:HD22	1:A:98:SER:HB2	1.76	0.49
2:Y:65:GLY:O	2:Y:71:MET:HG2	2.12	0.49
1:A:104:ARG:HB3	1:A:682:VAL:HG11	1.95	0.49
3:Z:131:LEU:HG	3:Z:139:VAL:HG11	1.94	0.49
1:A:657:MET:O	1:A:661:TYR:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:ILE:HG22	1:A:4:ASP:H	1.78	0.49
1:A:300:MET:O	1:A:301:LEU:HB2	2.11	0.49
1:A:503:GLU:O	1:A:505:ILE:HG22	2.12	0.49
1:A:746:LEU:O	1:A:747:GLN:HB2	2.12	0.49
2:Y:30:ASP:C	2:Y:31:ARG:HG3	2.37	0.49
3:Z:134:ASP:OD1	3:Z:136:GLU:N	2.46	0.49
1:A:706:GLY:C	1:A:708:PRO:HD3	2.38	0.49
2:Y:109:ILE:O	2:Y:113:LEU:HG	2.12	0.49
1:A:274:TYR:O	1:A:275:GLN:HG3	2.13	0.48
1:A:699:GLY:O	1:A:703:CYS:HB2	2.13	0.48
3:Z:4:SER:C	3:Z:6:ASP:N	2.71	0.48
1:A:796:LYS:HB2	3:Z:152:PRO:CG	2.42	0.48
1:A:829:LEU:HD11	2:Y:44:SER:HB2	1.95	0.48
3:Z:17:LEU:O	3:Z:20:PHE:HB3	2.14	0.48
1:A:134:ASP:HA	1:A:137:ILE:HD12	1.95	0.48
1:A:233:LYS:HE3	1:A:316:CYS:SG	2.53	0.48
1:A:815:ILE:HG21	2:Y:120:PHE:CE2	2.47	0.48
1:A:113:TYR:CD2	1:A:151:HIS:HA	2.49	0.48
1:A:466:ILE:HG23	1:A:587:VAL:HG13	1.94	0.48
2:Y:27:ILE:HG23	2:Y:35:VAL:CG2	2.43	0.48
2:Y:67:LEU:HG	2:Y:67:LEU:O	2.13	0.48
3:Z:4:SER:O	3:Z:8:ILE:HG13	2.13	0.48
3:Z:107:ARG:NH1	3:Z:107:ARG:HB2	2.28	0.48
1:A:244:GLY:HA3	1:A:265:TYR:HB2	1.96	0.48
1:A:410:VAL:CG1	1:A:411:THR:N	2.77	0.48
1:A:277:SER:O	1:A:278:ALA:HB3	2.12	0.48
1:A:453:ASN:HB3	1:A:454:TYR:CD1	2.49	0.48
1:A:88:MET:HE3	1:A:116:SER:HB2	1.95	0.48
1:A:489:ASN:HB3	1:A:512:PHE:HB3	1.96	0.48
1:A:648:VAL:HG12	1:A:649:HIS:N	2.29	0.48
1:A:676:LEU:C	1:A:678:GLN:N	2.72	0.48
1:A:182:LYS:HE3	1:A:462:ALA:HA	1.96	0.47
1:A:534:GLU:O	1:A:538:MET:HE3	2.14	0.47
1:A:690:GLN:C	1:A:694:ASN:HB2	2.39	0.47
1:A:780:LYS:HE2	1:A:784:MET:CE	2.44	0.47
2:Y:76:PHE:C	2:Y:78:ASP:H	2.22	0.47
1:A:78:ASN:ND2	1:A:98:SER:HB2	2.29	0.47
1:A:180:ALA:HA	1:A:672:ILE:CG2	2.41	0.47
1:A:43:PHE:CD1	1:A:97:ALA:HB2	2.49	0.47
1:A:45:SER:HA	1:A:77:MET:HE1	1.96	0.47
1:A:228:ALA:O	1:A:284:ILE:HB	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ILE:HG23	1:A:285:PHE:N	2.29	0.47
1:A:746:LEU:HD22	1:A:773:MET:HE1	1.97	0.47
1:A:237:ASN:OD1	1:A:238:ASN:N	2.47	0.47
1:A:411:THR:O	1:A:411:THR:HG22	2.15	0.47
1:A:415:ASN:OD1	1:A:418:GLN:HG3	2.15	0.47
1:A:275:GLN:OE1	1:A:312:ILE:HA	2.14	0.47
3:Z:70:PRO:O	3:Z:73:GLU:HG3	2.14	0.47
3:Z:100:PHE:HA	3:Z:139:VAL:O	2.14	0.47
3:Z:106:LEU:HD11	3:Z:110:LEU:HD11	1.95	0.47
1:A:125:PRO:O	1:A:126:TYR:HB2	2.14	0.47
1:A:141:ARG:HD2	1:A:196:VAL:HG12	1.97	0.47
1:A:672:ILE:HD13	1:A:672:ILE:N	2.28	0.47
1:A:676:LEU:C	1:A:678:GLN:H	2.22	0.47
1:A:736:LYS:O	1:A:740:GLU:HB2	2.15	0.47
1:A:787:ALA:HB1	3:Z:44:PRO:O	2.14	0.47
1:A:371:GLN:HE22	1:A:414:GLN:N	2.12	0.47
1:A:784:MET:HE1	3:Z:79:GLU:CD	2.40	0.47
1:A:790:ARG:O	1:A:794:ILE:HG12	2.14	0.47
1:A:567:LYS:HB3	1:A:568:PRO:CD	2.39	0.46
1:A:360:GLU:O	1:A:379:GLU:HG3	2.15	0.46
1:A:438:LEU:HD23	1:A:438:LEU:O	2.16	0.46
1:A:245:LYS:HE3	1:A:247:ILE:HB	1.98	0.46
1:A:816:ARG:O	1:A:820:VAL:HG23	2.15	0.46
3:Z:45:ARG:O	3:Z:48:ASP:HB2	2.15	0.46
1:A:36:VAL:O	1:A:43:PHE:HA	2.16	0.46
1:A:177:GLU:HB2	1:A:672:ILE:CD1	2.45	0.46
3:Z:11:LEU:HD23	3:Z:69:LEU:HD13	1.98	0.46
1:A:552:TYR:HA	1:A:556:MET:HB2	1.97	0.46
3:Z:43:ASN:N	3:Z:44:PRO:HD3	2.29	0.46
1:A:323:ASP:O	1:A:325:VAL:N	2.48	0.46
1:A:790:ARG:NH1	3:Z:46:ASN:OD1	2.48	0.46
2:Y:102:LYS:HA	2:Y:141:TYR:OH	2.16	0.46
1:A:12:TYR:HB2	1:A:131:ILE:CD1	2.45	0.46
1:A:163:MET:HE1	1:A:251:PHE:CG	2.51	0.46
1:A:361:MET:CE	1:A:383:VAL:HG21	2.46	0.46
1:A:403:VAL:CG1	1:A:404:LYS:N	2.79	0.46
1:A:822:ARG:CB	1:A:822:ARG:NH1	2.63	0.46
3:Z:4:SER:C	3:Z:6:ASP:H	2.24	0.46
1:A:782:ILE:O	1:A:786:GLN:HG3	2.16	0.46
1:A:266:LEU:HG	1:A:649:HIS:CE1	2.51	0.46
1:A:449:LYS:HD2	1:A:449:LYS:HA	1.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:108:HIS:O	3:Z:112:ALA:HB3	2.16	0.46
1:A:95:ASN:ND2	1:A:98:SER:H	2.14	0.45
1:A:308:LEU:HD12	1:A:308:LEU:O	2.16	0.45
1:A:414:GLN:HB2	1:A:418:GLN:CB	2.44	0.45
3:Z:35:ASP:HA	3:Z:38:ARG:HH11	1.80	0.45
1:A:157:ASP:C	1:A:159:ALA:N	2.74	0.45
1:A:275:GLN:HB2	1:A:314:GLN:HB2	1.98	0.45
1:A:653:LEU:CD2	1:A:657:MET:HG2	2.46	0.45
2:Y:22:GLU:C	2:Y:24:PHE:H	2.24	0.45
1:A:653:LEU:HD23	1:A:653:LEU:O	2.17	0.45
1:A:815:ILE:HD11	2:Y:144:PHE:CE1	2.51	0.45
3:Z:134:ASP:OD1	3:Z:134:ASP:C	2.59	0.45
1:A:505:ILE:HG23	1:A:505:ILE:O	2.16	0.45
1:A:179:GLY:HA2	4:A:996:SO4:O4	2.16	0.45
1:A:377:THR:HG22	1:A:381:GLU:CG	2.46	0.45
1:A:393:ASP:HB3	1:A:609:LEU:HD13	1.97	0.45
1:A:822:ARG:CG	1:A:822:ARG:NH1	2.74	0.45
2:Y:36:SER:C	2:Y:38:GLU:H	2.24	0.45
1:A:85:LEU:N	1:A:102:ASN:HD21	2.15	0.45
1:A:507:TRP:CH2	1:A:706:GLY:HA2	2.52	0.45
1:A:548:GLN:HG3	1:A:552:TYR:HE1	1.82	0.45
2:Y:24:PHE:CD2	2:Y:69:PHE:HB2	2.52	0.45
1:A:487:PHE:CZ	1:A:665:PRO:HG3	2.52	0.45
1:A:544:ASP:OD1	1:A:544:ASP:N	2.42	0.45
1:A:811:ILE:HG23	2:Y:93:PHE:CZ	2.51	0.45
2:Y:28:ASP:CG	2:Y:31:ARG:HA	2.42	0.45
2:Y:93:PHE:HB3	2:Y:141:TYR:CD2	2.51	0.45
1:A:15:VAL:CG1	1:A:16:ASP:N	2.80	0.45
1:A:309:TYR:CD2	1:A:356:LEU:HB3	2.52	0.45
1:A:371:GLN:HE21	1:A:371:GLN:HB2	1.66	0.45
2:Y:90:ARG:O	2:Y:90:ARG:CG	2.65	0.45
1:A:84:LYS:HA	1:A:106:ARG:HG3	1.99	0.44
1:A:273:THR:HG22	1:A:311:PHE:CE1	2.52	0.44
1:A:415:ASN:CG	1:A:418:GLN:HE21	2.24	0.44
1:A:795:ARG:HD3	3:Z:38:ARG:O	2.16	0.44
1:A:793:LEU:O	1:A:794:ILE:C	2.59	0.44
1:A:245:LYS:HE2	1:A:247:ILE:CG2	2.48	0.44
1:A:355:ILE:HG23	1:A:427:ALA:HB1	1.99	0.44
1:A:604:GLU:H	1:A:604:GLU:CD	2.24	0.44
1:A:827:TRP:CD1	1:A:827:TRP:C	2.95	0.44
1:A:663:THR:O	1:A:665:PRO:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:ARG:HD2	1:A:694:ASN:CG	2.43	0.44
1:A:560:ARG:HE	1:A:560:ARG:HB2	1.66	0.44
1:A:752:GLU:HG3	1:A:766:VAL:HG21	1.98	0.44
1:A:773:MET:HE3	1:A:773:MET:HB3	1.70	0.44
2:Y:89:ILE:C	2:Y:91:ASN:H	2.25	0.44
1:A:76:SER:HB3	1:A:93:TYR:CG	2.51	0.44
1:A:131:ILE:O	1:A:136:VAL:HG11	2.17	0.44
1:A:828:LYS:NZ	1:A:828:LYS:HB2	2.33	0.44
3:Z:131:LEU:HG	3:Z:139:VAL:CG1	2.47	0.44
1:A:300:MET:HE3	1:A:302:VAL:CG2	2.48	0.44
2:Y:93:PHE:CG	2:Y:141:TYR:HB2	2.53	0.44
2:Y:140:ASP:C	2:Y:140:ASP:OD1	2.61	0.44
1:A:600:ASP:O	1:A:600:ASP:CG	2.61	0.44
1:A:825:GLN:OE1	1:A:825:GLN:HA	2.16	0.44
2:Y:117:GLY:HA2	3:Z:20:PHE:CE1	2.53	0.44
3:Z:106:LEU:O	3:Z:110:LEU:HG	2.17	0.44
1:A:75:GLN:OE1	1:A:95:ASN:ND2	2.51	0.44
1:A:811:ILE:HD12	2:Y:93:PHE:CD1	2.53	0.44
3:Z:4:SER:OG	3:Z:6:ASP:HB3	2.17	0.44
1:A:470:ASN:OD1	1:A:587:VAL:HG13	2.18	0.43
1:A:760:VAL:O	1:A:760:VAL:HG13	2.18	0.43
1:A:763:LYS:O	1:A:766:VAL:HG23	2.17	0.43
3:Z:107:ARG:HB2	3:Z:107:ARG:HH11	1.83	0.43
1:A:377:THR:HG22	1:A:381:GLU:HG3	2.00	0.43
1:A:468:ASP:HB3	1:A:573:GLN:CA	2.38	0.43
1:A:491:HIS:CD2	1:A:495:LEU:HD11	2.52	0.43
1:A:827:TRP:O	1:A:831:SER:N	2.42	0.43
1:A:250:HIS:CB	1:A:452:ARG:HD3	2.48	0.43
1:A:251:PHE:HA	1:A:258:ALA:H	1.83	0.43
3:Z:31:PHE:CE2	3:Z:58:MET:HG2	2.53	0.43
3:Z:149:MET:HE2	3:Z:149:MET:HB3	1.88	0.43
1:A:500:TYR:HB3	1:A:505:ILE:O	2.18	0.43
2:Y:79:LYS:C	2:Y:81:SER:H	2.27	0.43
1:A:129:LEU:HA	1:A:130:PRO:HD3	1.78	0.43
1:A:148:ILE:CG1	1:A:149:PRO:HD2	2.27	0.43
1:A:361:MET:HE1	1:A:383:VAL:HG21	2.00	0.43
1:A:594:TRP:CD1	1:A:594:TRP:N	2.87	0.43
1:A:293:ILE:HD11	1:A:329:LYS:HG2	2.01	0.43
1:A:746:LEU:HD21	1:A:773:MET:CE	2.48	0.43
2:Y:102:LYS:C	2:Y:141:TYR:CE1	2.97	0.43
3:Z:25:ASP:OD2	3:Z:25:ASP:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:CYS:C	1:A:77:MET:HE3	2.44	0.43
1:A:401:PRO:CG	1:A:603:ASN:HD21	2.23	0.43
1:A:493:PHE:CD1	1:A:511:ASP:HA	2.53	0.43
1:A:287:GLN:HE21	1:A:327:GLU:HB3	1.84	0.43
1:A:415:ASN:ND2	1:A:418:GLN:HE21	2.17	0.43
1:A:722:ILE:HD11	3:Z:88:GLU:O	2.18	0.43
1:A:743:LEU:O	1:A:748:MET:HB2	2.18	0.43
1:A:766:VAL:C	1:A:768:GLY:N	2.73	0.43
1:A:824:TRP:CE2	1:A:826:TRP:HD1	2.37	0.43
3:Z:33:LEU:HA	3:Z:68:PHE:HZ	1.81	0.43
1:A:417:ASN:O	1:A:421:ASN:HB2	2.19	0.43
1:A:814:ASN:ND2	2:Y:89:ILE:HG12	2.34	0.43
1:A:35:TRP:CE2	1:A:77:MET:HE2	2.54	0.42
1:A:126:TYR:CE1	1:A:677:LYS:HA	2.54	0.42
1:A:416:MET:O	1:A:420:VAL:HG13	2.19	0.42
1:A:580:LEU:HD12	1:A:580:LEU:HA	1.86	0.42
2:Y:65:GLY:O	2:Y:66:PRO:C	2.61	0.42
1:A:777:ARG:HA	1:A:777:ARG:HD2	1.88	0.42
1:A:826:TRP:CZ2	2:Y:59:MET:SD	3.08	0.42
1:A:480:THR:C	1:A:482:GLU:N	2.77	0.42
1:A:691:LEU:CD2	1:A:696:VAL:HG21	2.47	0.42
3:Z:126:ILE:HG23	3:Z:131:LEU:HB3	2.01	0.42
2:Y:19:GLU:HA	2:Y:22:GLU:HB2	2.01	0.42
1:A:225:VAL:HG23	1:A:226:LEU:N	2.33	0.42
1:A:471:SER:OG	1:A:472:PHE:N	2.51	0.42
1:A:516:LEU:HD22	1:A:516:LEU:HA	1.91	0.42
1:A:720:TYR:O	1:A:742:ILE:HD13	2.20	0.42
2:Y:140:ASP:OD1	2:Y:142:VAL:N	2.53	0.42
3:Z:94:ASP:OD2	3:Z:97:GLY:HA2	2.20	0.42
3:Z:101:ILE:HG22	3:Z:141:TYR:CD1	2.54	0.42
1:A:16:ASP:HB3	1:A:19:LYS:CB	2.49	0.42
1:A:398:LEU:HD21	1:A:423:VAL:CG2	2.48	0.42
1:A:594:TRP:CD1	1:A:594:TRP:H	2.38	0.42
1:A:752:GLU:HG3	1:A:766:VAL:CG2	2.50	0.42
1:A:297:ASN:N	1:A:297:ASN:ND2	2.68	0.42
1:A:402:LYS:CB	1:A:605:ASN:ND2	2.82	0.42
1:A:828:LYS:O	1:A:832:LYS:HG3	2.19	0.42
2:Y:67:LEU:HA	2:Y:71:MET:HB3	2.01	0.42
3:Z:44:PRO:CG	3:Z:75:LEU:HD12	2.49	0.42
1:A:227:GLU:HG2	1:A:231:ASN:ND2	2.35	0.42
1:A:246:PHE:HB3	1:A:263:GLU:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:ILE:H	1:A:811:ILE:HG12	1.62	0.42
2:Y:103:LYS:N	2:Y:141:TYR:HE1	2.18	0.42
1:A:794:ILE:HD12	3:Z:35:ASP:OD2	2.20	0.42
1:A:518:MET:HE1	1:A:560:ARG:NH1	2.35	0.42
1:A:712:ILE:HA	1:A:759:LYS:CB	2.50	0.42
1:A:496:GLU:OE1	1:A:496:GLU:HA	2.20	0.41
1:A:587:VAL:HA	1:A:588:PRO:HD3	1.80	0.41
1:A:712:ILE:O	1:A:714:SER:N	2.53	0.41
1:A:768:GLY:O	1:A:771:GLU:HB2	2.19	0.41
1:A:177:GLU:HB2	1:A:672:ILE:HD11	2.02	0.41
1:A:283:HIS:O	1:A:287:GLN:HG3	2.20	0.41
1:A:514:MET:C	1:A:516:LEU:H	2.28	0.41
1:A:786:GLN:HE21	3:Z:110:LEU:HA	1.85	0.41
1:A:157:ASP:HB2	1:A:192:TYR:CZ	2.53	0.41
1:A:179:GLY:CA	4:A:996:SO4:O4	2.68	0.41
1:A:438:LEU:HD23	1:A:438:LEU:C	2.44	0.41
3:Z:3:LEU:CD2	3:Z:7:GLU:HG2	2.50	0.41
1:A:234:THR:O	1:A:236:ARG:N	2.52	0.41
1:A:434:MET:O	1:A:437:TRP:HB3	2.20	0.41
1:A:557:GLY:C	1:A:558:LYS:HG3	2.46	0.41
1:A:656:LEU:O	1:A:659:ASN:N	2.49	0.41
3:Z:57:LYS:HG2	3:Z:58:MET:N	2.36	0.41
3:Z:93:PHE:CE2	3:Z:109:VAL:HG22	2.55	0.41
1:A:323:ASP:C	1:A:325:VAL:H	2.28	0.41
1:A:821:LEU:HD11	1:A:827:TRP:CE3	2.56	0.41
2:Y:21:LYS:HB2	2:Y:69:PHE:CE1	2.55	0.41
2:Y:35:VAL:HG11	2:Y:40:ILE:HG13	2.02	0.41
1:A:88:MET:HB3	1:A:91:MET:HE2	2.03	0.41
1:A:131:ILE:HG22	1:A:151:HIS:HE2	1.86	0.41
1:A:401:PRO:O	1:A:411:THR:HA	2.20	0.41
1:A:367:PRO:HB2	1:A:369:GLU:HG2	2.03	0.41
1:A:486:GLN:HA	1:A:516:LEU:HD12	2.02	0.41
1:A:728:ILE:O	1:A:729:PRO:O	2.39	0.41
1:A:287:GLN:HB3	1:A:328:PHE:CG	2.56	0.41
1:A:400:LYS:N	1:A:401:PRO:HD3	2.36	0.41
1:A:598:ASN:ND2	1:A:644:THR:OG1	2.54	0.41
1:A:767:LEU:O	1:A:771:GLU:HG2	2.20	0.41
1:A:153:PHE:HB3	1:A:192:TYR:CE2	2.56	0.41
1:A:250:HIS:O	1:A:258:ALA:N	2.49	0.41
1:A:369:GLU:HG2	1:A:369:GLU:H	1.68	0.41
1:A:771:GLU:O	1:A:774:ARG:HB3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:796:LYS:HB2	3:Z:152:PRO:HG2	2.02	0.41
2:Y:90:ARG:O	2:Y:90:ARG:HG2	2.20	0.41
1:A:32:LYS:O	1:A:47:GLU:HA	2.21	0.41
1:A:121:ILE:H	1:A:121:ILE:HG13	1.56	0.41
1:A:175:THR:OG1	1:A:669:ARG:HD3	2.21	0.41
1:A:327:GLU:OE1	1:A:327:GLU:HA	2.21	0.41
2:Y:93:PHE:HD1	2:Y:104:LEU:HD11	1.86	0.41
1:A:12:TYR:HE2	1:A:127:ARG:NH2	2.19	0.40
1:A:323:ASP:C	1:A:325:VAL:N	2.79	0.40
1:A:333:GLU:O	1:A:337:ILE:HG13	2.21	0.40
1:A:530:LEU:O	1:A:534:GLU:HG3	2.21	0.40
2:Y:27:ILE:HD12	2:Y:27:ILE:HA	1.91	0.40
2:Y:35:VAL:O	2:Y:35:VAL:HG12	2.20	0.40
2:Y:75:ILE:O	2:Y:75:ILE:CG2	2.67	0.40
3:Z:101:ILE:HD11	3:Z:105:GLU:CG	2.51	0.40
1:A:280:ARG:HH12	1:A:324:ASP:CG	2.28	0.40
1:A:689:HIS:O	1:A:692:GLN:HB3	2.21	0.40
1:A:707:PHE:CE2	1:A:763:LYS:HE2	2.56	0.40
1:A:708:PRO:HB2	1:A:709:SER:H	1.72	0.40
3:Z:3:LEU:HD22	3:Z:7:GLU:HG2	2.04	0.40
3:Z:118:SER:O	3:Z:121:ASP:N	2.53	0.40
3:Z:143:ASP:O	3:Z:147:LYS:HG2	2.22	0.40
1:A:78:ASN:HA	1:A:79:PRO:HD3	1.95	0.40
1:A:464:PHE:HE2	1:A:466:ILE:HG12	1.86	0.40
1:A:777:ARG:O	1:A:778:LEU:C	2.65	0.40
2:Y:142:VAL:O	2:Y:145:THR:HB	2.21	0.40
1:A:88:MET:HG2	1:A:102:ASN:OD1	2.21	0.40
1:A:286:TYR:OH	1:A:312:ILE:HB	2.21	0.40
3:Z:16:GLU:O	3:Z:17:LEU:C	2.64	0.40
1:A:30:GLY:HA3	1:A:772:GLU:OE2	2.21	0.40
1:A:242:ARG:HA	1:A:242:ARG:HD2	1.72	0.40
1:A:337:ILE:O	1:A:337:ILE:HG22	2.20	0.40
1:A:505:ILE:HD11	1:A:754:ARG:HB3	2.02	0.40
1:A:824:TRP:HE3	1:A:827:TRP:HB2	1.87	0.40
2:Y:75:ILE:C	2:Y:76:PHE:HD1	2.30	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	794/840 (94%)	660 (83%)	113 (14%)	21 (3%)	4	21
2	Y	140/156 (90%)	111 (79%)	25 (18%)	4 (3%)	3	19
3	Z	153/156 (98%)	136 (89%)	11 (7%)	6 (4%)	2	14
All	All	1087/1152 (94%)	907 (83%)	149 (14%)	31 (3%)	3	19

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	PRO
1	A	625	PRO
1	A	708	PRO
1	A	713	TYR
1	A	834	LYS
2	Y	66	PRO
1	A	65	SER
1	A	235	THR
1	A	324	ASP
1	A	367	PRO
1	A	510	ILE
1	A	528	GLY
1	A	568	PRO
1	A	833	VAL
2	Y	85	SER
3	Z	25	ASP
3	Z	96	GLU
3	Z	116	ARG
3	Z	154	PRO
1	A	266	LEU
1	A	540	PRO
2	Y	119	ASN
3	Z	31	PHE
1	A	116	SER

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Mol	Chain	Res	Type
1	A	793	LEU
1	A	504	GLY
2	Y	64	PRO
3	Z	21	TRP
1	A	366	ARG
1	A	731	GLY
1	A	794	ILE

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	666/732 (91%)	559 (84%)	107 (16%)	2	11
2	Y	108/133 (81%)	79 (73%)	29 (27%)	0	2
3	Z	126/132 (96%)	106 (84%)	20 (16%)	2	12
All	All	900/997 (90%)	744 (83%)	156 (17%)	2	9

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASP
1	A	6	SER
1	A	8	PRO
1	A	51	SER
1	A	54	ASP
1	A	57	THR
1	A	67	ARG
1	A	94	LEU
1	A	95	ASN
1	A	102	ASN
1	A	104	ARG
1	A	114	THR
1	A	128	ARG
1	A	131	ILE
1	A	139	LYS

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Mol	Chain	Res	Type
1	A	158	ASN
1	A	161	GLN
1	A	162	ASN
1	A	188	LYS
1	A	195	LYS
1	A	214	SER
1	A	223	ASN
1	A	233	LYS
1	A	235	THR
1	A	270	SER
1	A	288	ILE
1	A	294	PRO
1	A	304	PRO
1	A	306	SER
1	A	308	LEU
1	A	314	GLN
1	A	326	GLU
1	A	327	GLU
1	A	341	THR
1	A	367	PRO
1	A	371	GLN
1	A	398	LEU
1	A	400	LYS
1	A	401	PRO
1	A	403	VAL
1	A	411	THR
1	A	415	ASN
1	A	420	VAL
1	A	421	ASN
1	A	442	VAL
1	A	444	LYS
1	A	448	THR
1	A	449	LYS
1	A	452	ARG
1	A	456	ILE
1	A	461	ILE
1	A	470	ASN
1	A	476	CYS
1	A	492	MET
1	A	505	ILE
1	A	507	TRP
1	A	514	MET

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Mol	Chain	Res	Type
1	A	516	LEU
1	A	526	PRO
1	A	527	MET
1	A	531	SER
1	A	533	LEU
1	A	544	ASP
1	A	560	ARG
1	A	565	PRO
1	A	568	PRO
1	A	571	PRO
1	A	575	PRO
1	A	586	ASN
1	A	595	LEU
1	A	600	ASP
1	A	601	PRO
1	A	603	ASN
1	A	616	PRO
1	A	623	LYS
1	A	644	THR
1	A	648	VAL
1	A	665	PRO
1	A	672	ILE
1	A	693	CYS
1	A	701	ARG
1	A	702	ILE
1	A	709	SER
1	A	712	ILE
1	A	718	GLN
1	A	729	PRO
1	A	730	GLN
1	A	734	ASP
1	A	740	GLU
1	A	741	LYS
1	A	750	PRO
1	A	752	GLU
1	A	757	THR
1	A	759	LYS
1	A	767	LEU
1	A	772	GLU
1	A	773	MET
1	A	781	ILE
1	A	782	ILE

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Mol	Chain	Res	Type
1	A	811	ILE
1	A	815	ILE
1	A	817	LYS
1	A	822	ARG
1	A	828	LYS
1	A	830	TYR
1	A	835	PRO
1	A	836	LEU
2	Y	16	GLN
2	Y	20	MET
2	Y	22	GLU
2	Y	25	SER
2	Y	26	MET
2	Y	27	ILE
2	Y	29	VAL
2	Y	31	ARG
2	Y	35	VAL
2	Y	36	SER
2	Y	43	ILE
2	Y	46	GLN
2	Y	51	PRO
2	Y	52	ASP
2	Y	53	ASP
2	Y	57	THR
2	Y	59	MET
2	Y	64	PRO
2	Y	66	PRO
2	Y	67	LEU
2	Y	68	ASN
2	Y	69	PHE
2	Y	74	SER
2	Y	77	SER
2	Y	90	ARG
2	Y	119	ASN
2	Y	122	LYS
2	Y	145	THR
2	Y	151	SER
3	Z	10	ASP
3	Z	12	LYS
3	Z	45	ARG
3	Z	58	MET
3	Z	62	SER

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Mol	Chain	Res	Type
3	Z	64	PRO
3	Z	67	GLU
3	Z	68	PHE
3	Z	69	LEU
3	Z	70	PRO
3	Z	77	ASP
3	Z	79	GLU
3	Z	80	GLN
3	Z	101	ILE
3	Z	107	ARG
3	Z	124	GLU
3	Z	127	LYS
3	Z	139	VAL
3	Z	146	LYS
3	Z	152	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	95	ASN
1	A	102	ASN
1	A	158	ASN
1	A	287	GLN
1	A	291	ASN
1	A	297	ASN
1	A	321	ASN
1	A	371	GLN
1	A	414	GLN
1	A	418	GLN
1	A	436	ASN
1	A	453	ASN
1	A	470	ASN
1	A	485	GLN
1	A	486	GLN
1	A	489	ASN
1	A	491	HIS
1	A	497	GLN
1	A	517	GLN
1	A	586	ASN
1	A	603	ASN
1	A	649	HIS

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Mol	Chain	Res	Type
1	A	659	ASN
1	A	718	GLN
1	A	769	ASN
1	A	814	ASN
2	Y	16	GLN
2	Y	46	GLN
2	Y	91	ASN
3	Z	5	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are 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	SO4	A	996	-	4,4,4	0.36	0	6,6,6	0.09	0
5	ADP	A	995	-	28,29,29	1.64	5 (17%)	43,45,45	2.00	9 (20%)

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
5	ADP	A	995	-	-	9/16/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	995	ADP	C5-N7	-4.48	1.30	1.39
5	A	995	ADP	PA-O3A	-3.06	1.56	1.59
5	A	995	ADP	C1'-N9	2.71	1.53	1.46
5	A	995	ADP	C5-C4	2.50	1.43	1.39
5	A	995	ADP	C4-N3	2.29	1.38	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	995	ADP	N3-C2-N1	-6.67	118.48	128.58
5	A	995	ADP	C5-C4-N3	-5.45	119.22	126.72
5	A	995	ADP	C2-N3-C4	4.44	122.69	111.83
5	A	995	ADP	N3-C4-N9	4.26	134.41	127.17
5	A	995	ADP	C5-N7-C8	3.36	108.73	103.45
5	A	995	ADP	C4-C5-N7	-2.64	107.57	110.58
5	A	995	ADP	N9-C8-N7	-2.43	110.49	113.94
5	A	995	ADP	O3B-PB-O3A	2.06	111.53	104.64
5	A	995	ADP	C2-N1-C6	2.02	122.04	118.73

There are no chirality outliers.

All (9) torsion outliers are listed below:

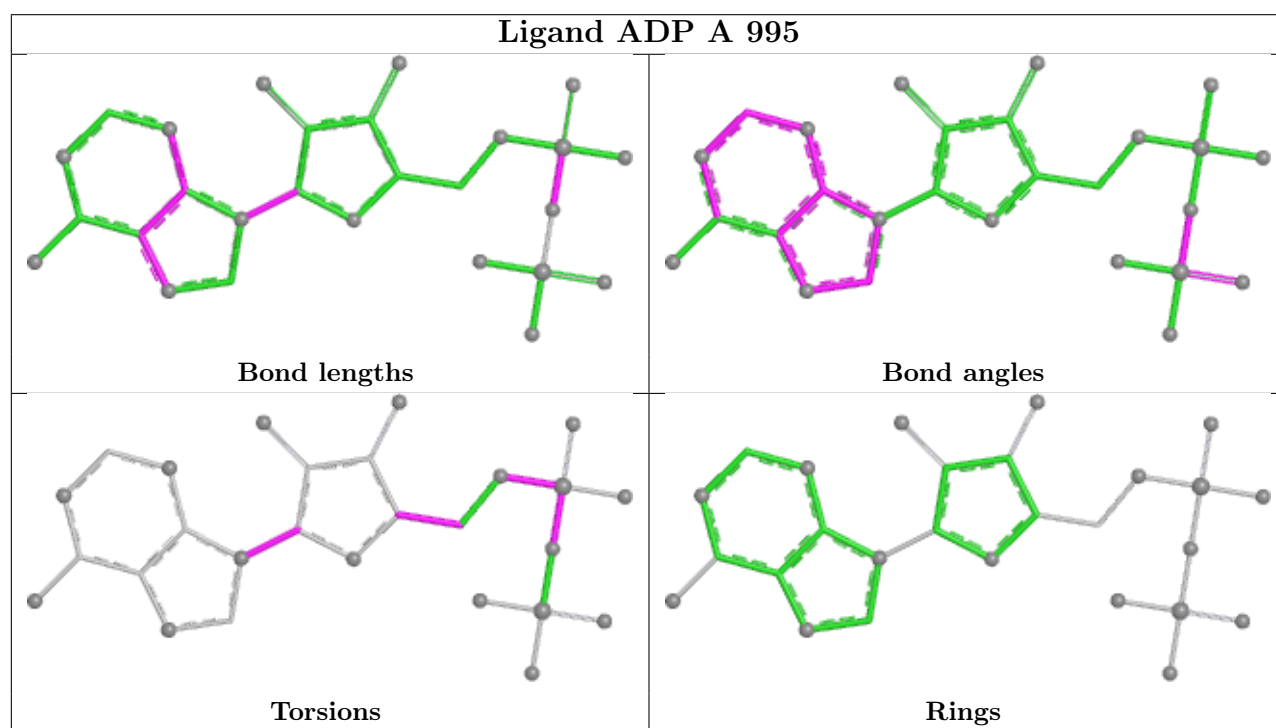
Mol	Chain	Res	Type	Atoms
5	A	995	ADP	C5'-O5'-PA-O1A
5	A	995	ADP	C5'-O5'-PA-O2A
5	A	995	ADP	C5'-O5'-PA-O3A
5	A	995	ADP	O4'-C4'-C5'-O5'
5	A	995	ADP	C3'-C4'-C5'-O5'
5	A	995	ADP	C2'-C1'-N9-C4
5	A	995	ADP	PB-O3A-PA-O1A
5	A	995	ADP	C2'-C1'-N9-C8
5	A	995	ADP	PB-O3A-PA-O2A

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	996	SO4	3	0
5	A	995	ADP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	802/840 (95%)	-0.26	2 (0%) 91 83	33, 72, 134, 176	0
2	Y	142/156 (91%)	0.08	3 (2%) 63 42	34, 126, 187, 201	0
3	Z	155/156 (99%)	-0.40	0 100 100	31, 67, 104, 126	0
All	All	1099/1152 (95%)	-0.23	5 (0%) 87 73	31, 72, 161, 201	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Y	27	ILE	2.8
2	Y	72	PHE	2.4
1	A	461	ILE	2.3
1	A	460	ASP	2.2
2	Y	13	PRO	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](#)

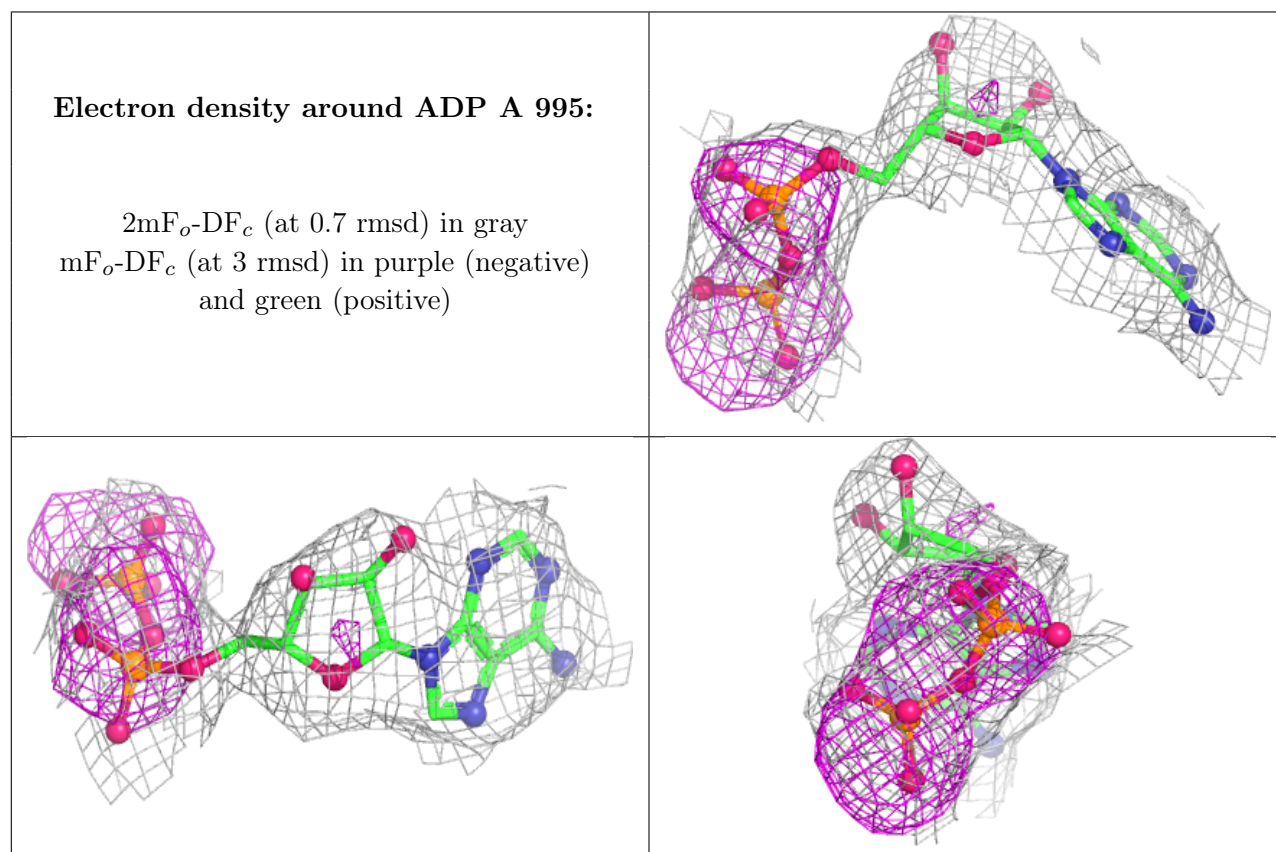
There are no oligosaccharides in this entry.

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
5	ADP	A	995	27/27	0.74	0.12	53,79,92,102	0
6	MG	Y	999	1/1	0.81	0.06	137,137,137,137	0
4	SO4	A	996	5/5	0.90	0.10	54,73,84,84	0
7	CA	Z	998	1/1	0.99	0.15	75,75,75,75	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 ⓘ

There are no such residues in this entry.