Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:34 pm BST

PDB ID	:	3UA3
Title	:	Crystal Structure of Protein Arginine Methyltransferase PRMT5 in complex with SAH
Authors	:	Sun, L.; Wang, M.; Lv, Z.; Yang, N.; Liu, Y.; Bao, S.; Gong, W.; Xu, R.M.
Deposited on	:	2011-10-20
Resolution	:	3.00 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 following versions of software and data (see references ⓘ) were used in the production of this report:

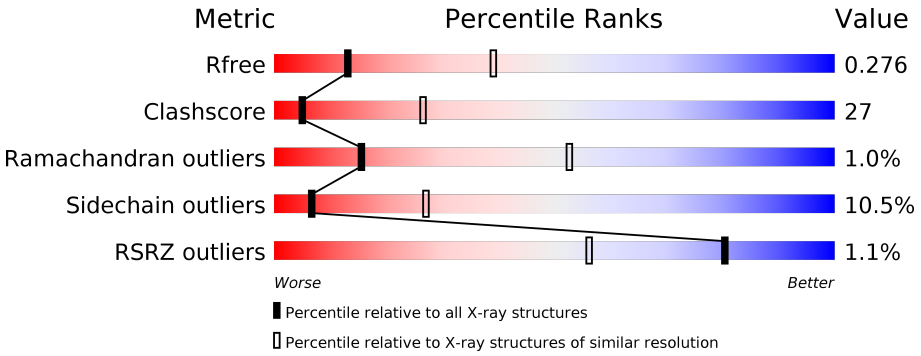
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	745	% 47% 37% 5% 11%
1	B	745	% 47% 35% 6% 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10737 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.

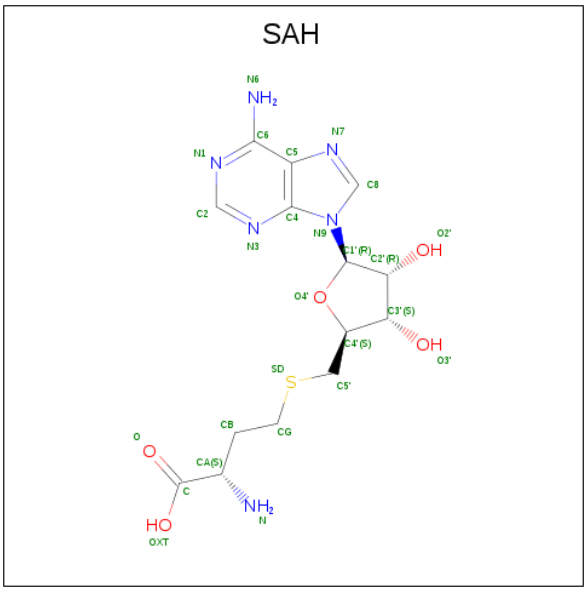
- Molecule 1 is a protein called Protein arginine N-methyltransferase 5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	662	Total	C	N	O	S	Se	1	0	0
			5314	3400	901	993	6	14			
1	B	651	Total	C	N	O	S	Se	1	0	0
			5225	3350	881	974	6	14			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MSE	-	EXPRESSION TAG	UNP P46580
A	-1	ALA	-	EXPRESSION TAG	UNP P46580
A	0	SER	-	EXPRESSION TAG	UNP P46580
A	735	LEU	-	EXPRESSION TAG	UNP P46580
A	736	GLU	-	EXPRESSION TAG	UNP P46580
A	737	HIS	-	EXPRESSION TAG	UNP P46580
A	738	HIS	-	EXPRESSION TAG	UNP P46580
A	739	HIS	-	EXPRESSION TAG	UNP P46580
A	740	HIS	-	EXPRESSION TAG	UNP P46580
A	741	HIS	-	EXPRESSION TAG	UNP P46580
A	742	HIS	-	EXPRESSION TAG	UNP P46580
B	-2	MSE	-	EXPRESSION TAG	UNP P46580
B	-1	ALA	-	EXPRESSION TAG	UNP P46580
B	0	SER	-	EXPRESSION TAG	UNP P46580
B	735	LEU	-	EXPRESSION TAG	UNP P46580
B	736	GLU	-	EXPRESSION TAG	UNP P46580
B	737	HIS	-	EXPRESSION TAG	UNP P46580
B	738	HIS	-	EXPRESSION TAG	UNP P46580
B	739	HIS	-	EXPRESSION TAG	UNP P46580
B	740	HIS	-	EXPRESSION TAG	UNP P46580
B	741	HIS	-	EXPRESSION TAG	UNP P46580
B	742	HIS	-	EXPRESSION TAG	UNP P46580

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

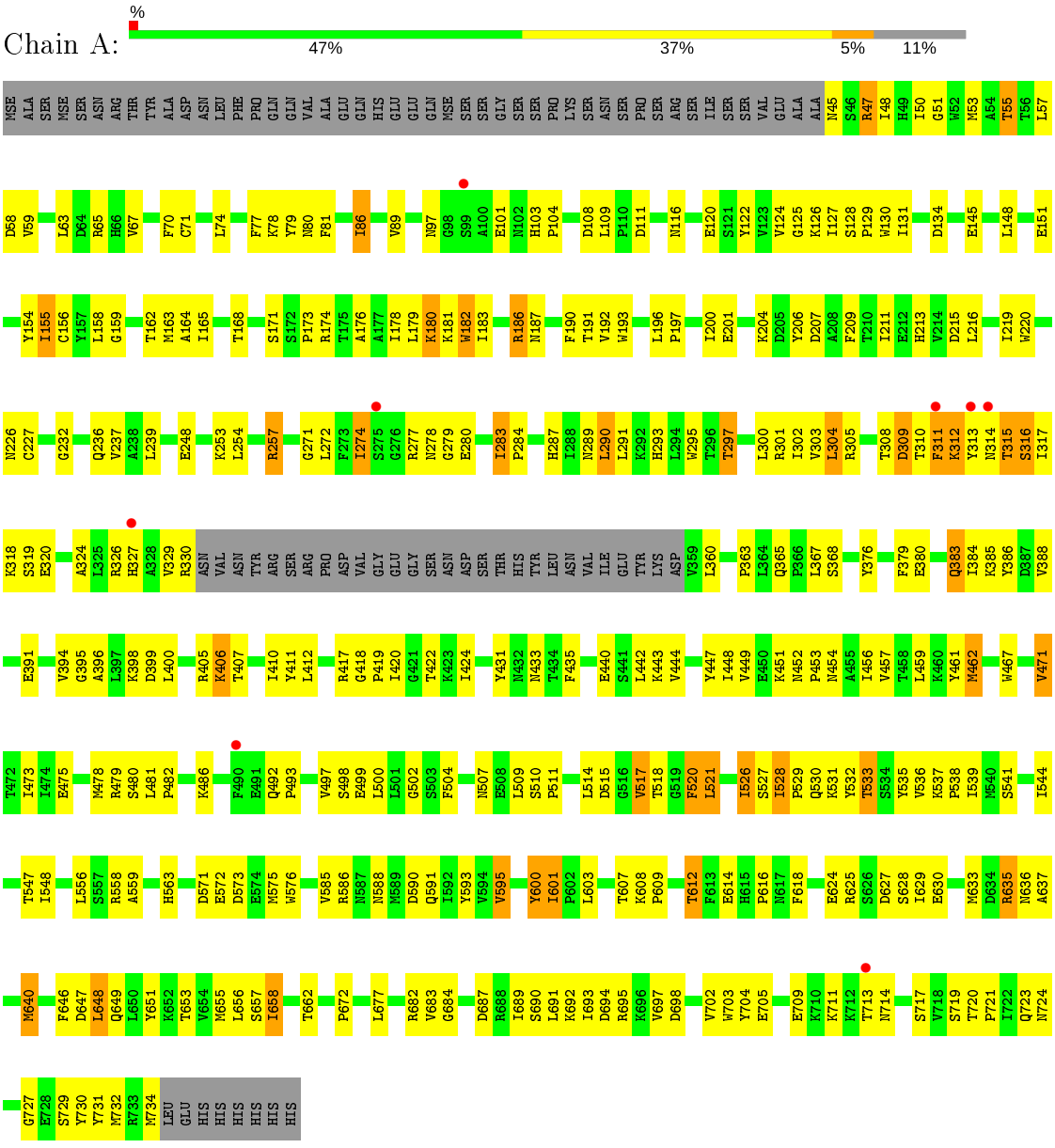
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	79	Total	O	0	0
			79	79		
3	B	67	Total	O	0	0
			67	67		

3 Residue-property plots (i)

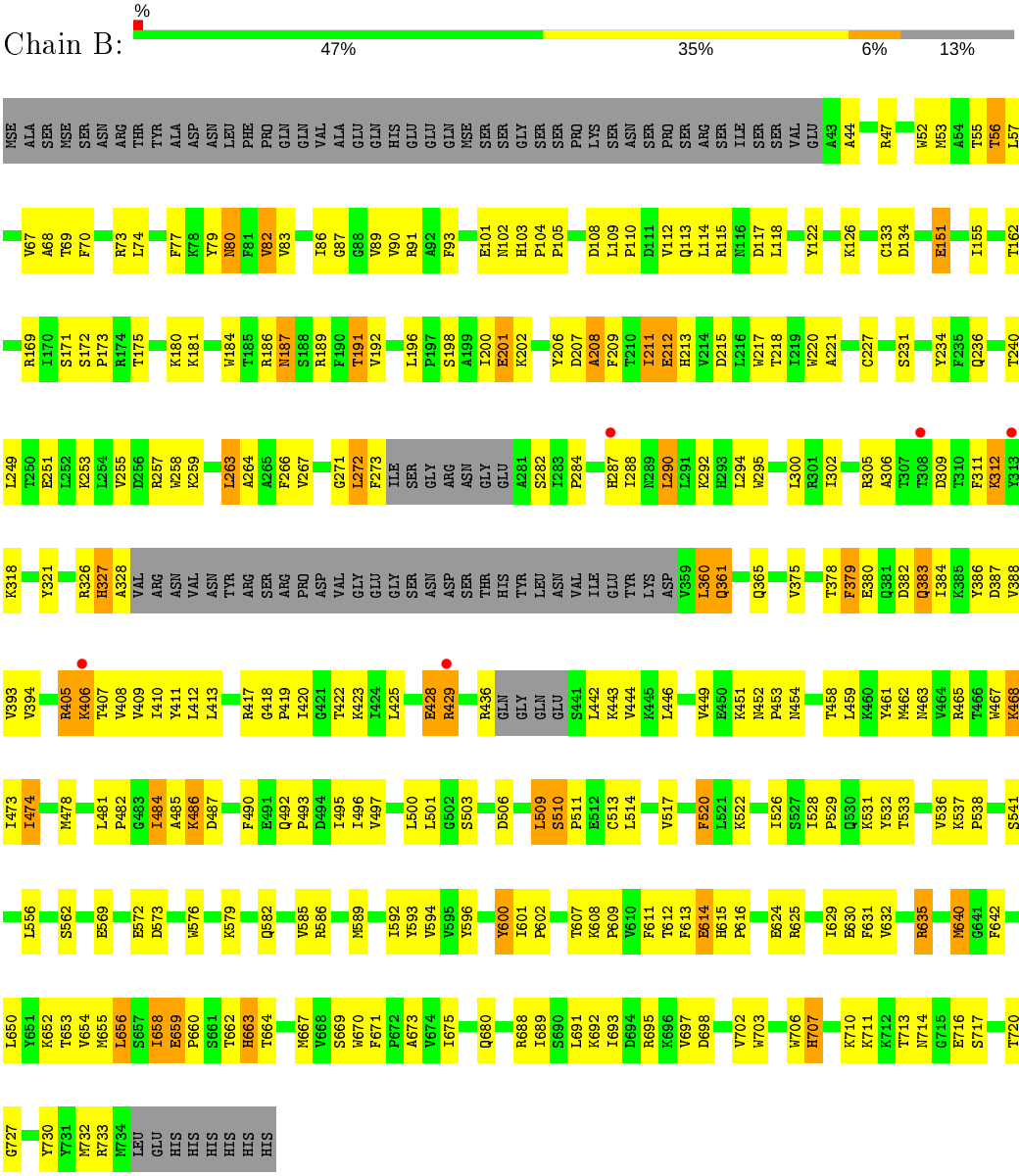
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Protein arginine N-methyltransferase 5



- Molecule 1: Protein arginine N-methyltransferase 5

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	100.38Å 129.38Å 149.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.95 – 3.00 29.95 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.95-3.00) 100.0 (29.95-3.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.41 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.223 , 0.281 0.218 , 0.276	Depositor DCC
R_{free} test set	1828 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å^2)	38.8	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 69.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	10737	wwPDB-VP
Average B, all atoms (Å^2)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SAH

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	0.31	0/5433	0.51	0/7360
1	B	0.30	0/5342	0.50	0/7237
All	All	0.31	0/10775	0.50	0/14597

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	5314	0	5259	294	0
1	B	5225	0	5173	285	0
2	A	26	0	19	3	0
2	B	26	0	19	0	0
3	A	79	0	0	3	0
3	B	67	0	0	6	0
All	All	10737	0	10470	572	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 27.

All (572) 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:74:LEU:HB3	1:A:79:TYR:HE1	1.22	1.02
1:A:635:ARG:HH11	1:A:635:ARG:HG2	1.23	1.02
1:B:57:LEU:HD12	1:B:306:ALA:HB1	1.43	0.96
1:A:449:VAL:HG21	1:A:481:LEU:HD11	1.48	0.94
1:A:422:THR:HG22	1:A:467:TRP:HE1	1.32	0.94
1:A:601:ILE:HD11	1:B:259:LYS:HE3	1.48	0.92
1:A:74:LEU:HB3	1:A:79:TYR:CE1	2.05	0.92
1:A:277:ARG:HB2	1:A:280:GLU:HG2	1.53	0.91
1:B:198:SER:HB2	1:B:202:LYS:HD3	1.54	0.89
1:A:313:TYR:HD2	1:A:316:SER:HB3	1.36	0.88
1:A:312:LYS:HB3	1:A:317:ILE:HG22	1.53	0.87
1:B:266:PHE:HB2	1:B:302:ILE:HG12	1.55	0.86
1:B:312:LYS:HB3	1:B:317:ILE:HB	1.56	0.86
1:B:692:LYS:HB2	1:B:707:HIS:CD2	2.14	0.83
1:B:511:PRO:HG3	1:B:532:TYR:OH	1.77	0.83
1:B:724:ASN:HD21	1:B:730:TYR:HB3	1.44	0.83
1:B:273:PHE:C	1:B:282:SER:H	1.83	0.83
1:B:635:ARG:HG2	1:B:635:ARG:HH11	1.44	0.81
1:B:390:GLY:HA3	1:B:423:LYS:HE2	1.60	0.81
1:A:630:GLU:HA	1:A:689:ILE:O	1.81	0.80
1:A:532:TYR:HB3	1:A:648:LEU:HB2	1.63	0.80
1:B:87:GLY:HA3	1:B:91:ARG:HD3	1.64	0.79
1:B:500:LEU:HB2	1:B:510:SER:HB2	1.63	0.78
1:B:77:PHE:CD2	1:B:318:LYS:HD3	2.18	0.78
1:A:313:TYR:CD2	1:A:316:SER:HB3	2.18	0.78
1:B:70:PHE:HE2	1:B:74:LEU:HD11	1.48	0.77
1:B:70:PHE:CE2	1:B:74:LEU:HD11	2.19	0.77
1:A:272:LEU:HD21	1:A:283:ILE:HA	1.66	0.77
1:A:411:TYR:HD2	1:A:493:PRO:HB3	1.49	0.77
1:A:312:LYS:HB3	1:A:317:ILE:CG2	2.14	0.76
1:A:608:LYS:HG3	1:A:609:PRO:HD2	1.68	0.76
1:A:376:TYR:HB3	1:A:417:ARG:HD2	1.67	0.76
1:A:411:TYR:CD2	1:A:493:PRO:HB3	2.20	0.76
1:B:724:ASN:ND2	1:B:730:TYR:HB3	2.00	0.75
1:B:74:LEU:HB3	1:B:79:TYR:CE1	2.23	0.74
1:B:86:ILE:HD13	1:B:155:ILE:HG12	1.70	0.74
1:A:635:ARG:NH1	1:A:635:ARG:HG2	1.90	0.74
1:B:698:ASP:HB2	1:B:703:TRP:HZ3	1.51	0.74
1:B:411:TYR:CD2	1:B:493:PRO:HB3	2.23	0.73
1:A:531:LYS:HB3	1:A:649:GLN:HG2	1.70	0.73
1:B:541:SER:HB2	1:B:600:TYR:HB2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:635:ARG:CG	1:A:635:ARG:HH11	2.00	0.73
1:B:659:GLU:O	1:B:663:HIS:HB2	1.89	0.73
1:B:240:THR:HA	1:B:267:VAL:HB	1.70	0.72
1:B:55:THR:HG22	1:B:57:LEU:H	1.54	0.72
1:A:317:ILE:HG13	1:A:320:GLU:OE1	1.89	0.72
1:A:47:ARG:HG2	1:A:48:ILE:HD12	1.70	0.72
1:A:53:MSE:HE3	1:A:303:VAL:HG11	1.71	0.72
1:B:648:LEU:CD2	1:B:656:LEU:HG	2.20	0.71
1:B:215:ASP:HB2	1:B:248:GLU:OE1	1.91	0.71
1:B:537:LYS:HE2	1:B:602:PRO:HB3	1.72	0.71
1:B:68:ALA:HB2	1:B:114:LEU:HD13	1.74	0.70
1:B:77:PHE:HD2	1:B:318:LYS:HD3	1.54	0.70
1:A:324:ALA:HA	1:A:327:HIS:CE1	2.26	0.70
1:B:74:LEU:HB3	1:B:79:TYR:HE1	1.54	0.70
1:B:86:ILE:HD11	1:B:151:GLU:HG2	1.74	0.70
1:B:449:VAL:HA	1:B:474:ILE:HG23	1.74	0.69
1:B:536:VAL:HG22	1:B:642:PHE:HB3	1.74	0.69
1:B:212:GLU:HG3	1:B:213:HIS:H	1.58	0.69
1:B:509:LEU:HD21	1:B:732:MSE:CB	2.22	0.69
1:B:59:VAL:HG13	1:B:89:VAL:HG11	1.73	0.69
1:A:155:ILE:HD12	1:A:163:MSE:HG3	1.75	0.69
1:B:189:ARG:HB3	1:B:234:TYR:HE1	1.56	0.69
1:B:405:ARG:HH21	1:B:405:ARG:HB2	1.56	0.69
1:B:284:PRO:HG2	1:B:287:HIS:CG	2.27	0.69
1:B:635:ARG:HG2	1:B:635:ARG:NH1	2.03	0.69
1:A:300:LEU:HD12	1:A:300:LEU:H	1.58	0.68
1:B:103:HIS:HB3	1:B:104:PRO:HD2	1.75	0.68
1:B:492:GLN:HB3	1:B:522:LYS:HG3	1.75	0.68
1:B:692:LYS:HB2	1:B:707:HIS:HD2	1.58	0.68
1:A:572:GLU:HG2	1:A:573:ASP:OD1	1.93	0.68
1:A:649:GLN:HA	1:A:655:MSE:HB3	1.75	0.68
1:B:86:ILE:HD13	1:B:155:ILE:CG1	2.25	0.67
1:A:317:ILE:O	1:A:317:ILE:HG12	1.93	0.67
1:B:649:GLN:HA	1:B:655:MSE:HB3	1.75	0.67
1:A:127:ILE:HG23	1:A:131:ILE:HD12	1.75	0.67
1:A:47:ARG:HH21	1:A:330:ARG:HD3	1.58	0.66
1:B:227:CYS:HB2	3:B:796:HOH:O	1.95	0.66
1:B:600:TYR:O	1:B:601:ILE:HD12	1.95	0.66
1:B:428:GLU:HG3	1:B:429:ARG:N	2.10	0.66
1:B:360:LEU:HD11	1:B:547:THR:HG22	1.76	0.66
1:A:48:ILE:HG21	1:A:326:ARG:HG2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:ARG:HH11	1:B:442:LEU:HB2	1.62	0.65
1:A:682:ARG:HH21	1:B:221:ALA:HB1	1.61	0.65
1:A:498:SER:O	1:A:529:PRO:HD3	1.97	0.65
1:A:308:THR:OG1	1:A:310:THR:HG22	1.97	0.65
1:A:544:ILE:HB	1:A:640:MSE:HE2	1.76	0.65
1:B:312:LYS:N	1:B:312:LYS:HD2	2.12	0.65
1:A:497:VAL:HG22	1:A:528:ILE:HG23	1.79	0.65
1:B:537:LYS:HB2	1:B:607:THR:HG22	1.78	0.65
1:A:179:LEU:O	1:A:183:ILE:HG12	1.97	0.64
1:A:254:LEU:O	1:A:257:ARG:HD3	1.98	0.64
1:B:418:GLY:N	1:B:419:PRO:HD3	2.12	0.64
1:A:86:ILE:HG21	1:A:155:ILE:CD1	2.28	0.64
1:B:70:PHE:O	1:B:74:LEU:HG	1.98	0.64
1:B:711:LYS:HA	1:B:716:GLU:O	1.98	0.64
1:B:407:THR:HA	1:B:443:LYS:O	1.98	0.64
1:A:649:GLN:HA	1:A:655:MSE:CB	2.28	0.63
1:B:380:GLU:HG2	1:B:419:PRO:HG2	1.81	0.63
1:A:400:LEU:HD22	1:A:405:ARG:HE	1.63	0.63
1:B:389:TYR:O	1:B:393:VAL:HG23	1.98	0.63
1:B:312:LYS:HD2	1:B:312:LYS:H	1.64	0.63
1:B:458:THR:O	1:B:462:MSE:HB2	1.98	0.63
1:A:272:LEU:HD11	1:A:284:PRO:HD3	1.81	0.63
1:B:201:GLU:HA	1:B:206:TYR:CD2	2.34	0.63
1:A:283:ILE:HG22	1:A:287:HIS:CB	2.29	0.63
1:A:517:VAL:HG13	1:A:521:LEU:HD21	1.81	0.63
1:B:189:ARG:HB3	1:B:234:TYR:CE1	2.32	0.63
1:B:541:SER:HB2	1:B:600:TYR:CB	2.28	0.62
1:A:127:ILE:CG2	1:A:131:ILE:HD12	2.29	0.62
1:B:532:TYR:CE1	1:B:613:PHE:HB2	2.35	0.62
1:B:496:ILE:HG13	1:B:496:ILE:O	1.99	0.62
1:A:422:THR:CG2	1:A:467:TRP:HE1	2.10	0.62
1:A:376:TYR:CB	1:A:417:ARG:HD2	2.30	0.62
1:B:422:THR:HG22	1:B:467:TRP:HE1	1.65	0.62
1:A:70:PHE:CZ	1:A:74:LEU:HD11	2.35	0.62
1:B:201:GLU:HA	1:B:206:TYR:CE2	2.34	0.62
1:B:509:LEU:HD21	1:B:732:MSE:HB3	1.82	0.62
1:A:86:ILE:HG12	1:A:86:ILE:O	2.00	0.61
1:A:86:ILE:HG21	1:A:155:ILE:HD11	1.83	0.61
1:B:412:LEU:HD21	1:B:420:ILE:HG23	1.83	0.61
1:B:509:LEU:HD21	1:B:732:MSE:HB2	1.82	0.61
1:A:220:TRP:CE3	1:A:237:VAL:HB	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:688:ARG:NH1	1:B:711:LYS:HD2	2.15	0.61
1:B:86:ILE:HG21	1:B:155:ILE:HD13	1.81	0.61
1:A:310:THR:C	1:A:312:LYS:N	2.52	0.61
1:B:56:THR:HA	1:B:59:VAL:HG23	1.81	0.61
1:A:310:THR:HG23	1:A:310:THR:O	1.99	0.61
1:B:463:ASN:HA	1:B:467:TRP:HB2	1.81	0.61
1:A:537:LYS:HD3	1:A:607:THR:HG22	1.82	0.60
1:A:406:LYS:HD2	1:A:406:LYS:H	1.65	0.60
1:A:47:ARG:H	1:A:47:ARG:HD2	1.66	0.60
1:A:313:TYR:HD2	1:A:316:SER:CB	2.13	0.60
1:B:459:LEU:HB3	1:B:473:ILE:HD12	1.82	0.60
1:A:530:GLN:HG3	1:A:651:TYR:HA	1.84	0.60
1:B:387:ASP:O	1:B:391:GLU:HG2	2.02	0.60
1:B:69:THR:O	1:B:73:ARG:HG3	2.01	0.60
1:A:181:LYS:HD2	1:A:576:TRP:CZ2	2.37	0.60
1:B:236:GLN:HB3	1:B:264:ALA:HB2	1.83	0.60
1:A:647:ASP:HB2	1:A:657:SER:HB2	1.84	0.59
1:B:461:TYR:CE2	1:B:465:ARG:HG3	2.37	0.59
1:B:245:LEU:HD13	1:B:287:HIS:NE2	2.18	0.59
1:B:635:ARG:HH11	1:B:635:ARG:CG	2.14	0.59
1:A:528:ILE:HA	1:A:529:PRO:C	2.23	0.59
1:B:258:TRP:HB3	1:B:263:LEU:HD22	1.83	0.59
1:A:646:PHE:H	1:A:658:ILE:HG22	1.66	0.59
1:A:57:LEU:HD13	1:A:309:ASP:HA	1.85	0.58
1:A:510:SER:HB3	1:A:511:PRO:HD3	1.84	0.58
1:A:720:THR:HB	1:A:721:PRO:HD2	1.85	0.58
1:B:86:ILE:HD13	1:B:155:ILE:CD1	2.34	0.58
1:B:326:ARG:C	1:B:328:ALA:H	2.07	0.58
1:B:410:ILE:HG13	1:B:495:ILE:HB	1.86	0.58
1:A:360:LEU:HD11	1:A:548:ILE:HA	1.86	0.58
1:B:375:VAL:O	1:B:379:PHE:HB2	2.03	0.58
1:B:562:SER:HB2	3:B:786:HOH:O	2.03	0.58
1:B:536:VAL:HG22	1:B:642:PHE:CB	2.33	0.58
1:A:363:PRO:HG2	1:A:730:TYR:OH	2.03	0.58
1:A:500:LEU:O	1:A:510:SER:HB2	2.04	0.57
1:A:637:ALA:HA	1:B:217:TRP:CH2	2.39	0.57
1:B:624:GLU:O	1:B:625:ARG:HD3	2.04	0.57
1:A:78:LYS:HE2	1:A:326:ARG:NH1	2.19	0.57
1:A:418:GLY:N	1:A:419:PRO:HD3	2.19	0.57
1:A:274:ILE:H	1:A:274:ILE:HD13	1.69	0.57
1:A:120:GLU:HG2	1:A:159:GLY:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:697:VAL:HG13	1:B:702:VAL:HG22	1.87	0.57
1:A:703:TRP:HE1	1:A:705:GLU:HG3	1.68	0.56
1:A:206:TYR:HE2	1:A:211:ILE:HD13	1.70	0.56
1:A:220:TRP:CD2	1:A:237:VAL:HB	2.40	0.56
1:B:86:ILE:CD1	1:B:155:ILE:HG12	2.35	0.56
1:A:289:ASN:O	1:A:293:HIS:HB2	2.06	0.56
1:B:208:ALA:HA	1:B:211:ILE:CD1	2.35	0.56
1:A:628:SER:O	1:A:629:ILE:HD13	2.04	0.56
1:A:376:TYR:O	1:A:379:PHE:HB2	2.06	0.56
1:A:502:GLY:HA3	1:A:507:ASN:OD1	2.06	0.56
1:A:695:ARG:HG3	1:A:704:TYR:HE2	1.70	0.56
1:B:52:TRP:HB2	1:B:79:TYR:CE1	2.40	0.56
1:A:310:THR:C	1:A:312:LYS:H	2.08	0.56
1:B:63:LEU:HD11	1:B:70:PHE:CD1	2.41	0.56
1:A:467:TRP:CE3	1:A:471:VAL:HG11	2.41	0.56
1:A:633:MSE:HG2	1:A:683:VAL:HG21	1.87	0.56
1:B:492:GLN:HB2	1:B:522:LYS:HE2	1.88	0.56
1:A:311:PHE:O	1:A:312:LYS:HB2	2.06	0.56
1:B:422:THR:HG22	1:B:467:TRP:NE1	2.21	0.56
1:B:646:PHE:HZ	1:B:670:TRP:CE3	2.24	0.56
1:A:380:GLU:HA	1:A:386:TYR:HE2	1.71	0.55
1:A:383:GLN:CD	1:A:383:GLN:H	2.08	0.55
1:A:478:MSE:HE3	2:A:743:SAH:C2	2.36	0.55
1:B:532:TYR:OH	1:B:615:HIS:HE1	1.89	0.55
1:B:659:GLU:HG3	1:B:660:PRO:N	2.21	0.55
1:A:196:LEU:HD12	1:A:239:LEU:HD23	1.87	0.55
1:A:563:HIS:HD2	1:A:591:GLN:OE1	1.89	0.55
1:A:406:LYS:HD2	1:A:407:THR:H	1.72	0.55
1:B:86:ILE:HD13	1:B:155:ILE:HD11	1.89	0.55
1:B:689:ILE:HD11	1:B:710:LYS:HG3	1.89	0.55
1:B:412:LEU:CD2	1:B:420:ILE:HG23	2.37	0.55
1:A:406:LYS:H	1:A:406:LYS:CD	2.19	0.54
1:A:451:LYS:HG3	1:A:452:ASN:N	2.22	0.54
1:B:86:ILE:HG21	1:B:155:ILE:CD1	2.37	0.54
1:B:653:THR:HG23	1:B:654:VAL:H	1.72	0.54
1:B:503:SER:HB3	1:B:671:PHE:O	2.07	0.54
1:B:181:LYS:HD2	1:B:576:TRP:CZ2	2.42	0.54
1:A:396:ALA:HB1	1:A:526:ILE:HD11	1.88	0.54
1:A:50:ILE:O	1:A:79:TYR:HB2	2.08	0.54
1:B:134:ASP:OD1	1:B:173:PRO:HD2	2.07	0.54
1:B:382:ASP:CG	1:B:669:SER:HB2	2.28	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:LYS:HB2	1:A:227:CYS:HA	1.88	0.54
1:A:196:LEU:HB3	1:A:197:PRO:HD2	1.89	0.54
1:A:81:PHE:HB2	1:A:122:TYR:O	2.06	0.54
1:B:428:GLU:HG3	1:B:429:ARG:H	1.71	0.54
1:A:305:ARG:HH11	1:A:305:ARG:HG2	1.73	0.54
1:A:274:ILE:HG12	1:A:274:ILE:O	2.07	0.54
1:B:649:GLN:HA	1:B:655:MSE:CB	2.38	0.54
1:A:63:LEU:HD11	1:A:70:PHE:CD1	2.43	0.54
1:B:391:GLU:O	1:B:394:VAL:HG22	2.08	0.54
1:B:405:ARG:HD3	1:B:405:ARG:H	1.71	0.54
1:B:77:PHE:CE2	1:B:318:LYS:HD3	2.43	0.54
1:B:406:LYS:HD2	1:B:407:THR:HG22	1.90	0.54
1:B:648:LEU:HD21	1:B:656:LEU:HG	1.90	0.54
1:A:533:THR:HB	1:A:612:THR:HG22	1.89	0.53
1:A:507:ASN:O	1:A:732:MSE:SE	2.76	0.53
1:B:89:VAL:HG13	1:B:93:PHE:CD2	2.42	0.53
1:B:187:ASN:N	1:B:187:ASN:OD1	2.41	0.53
1:B:468:LYS:HE3	1:B:468:LYS:HA	1.89	0.53
1:A:151:GLU:O	1:A:155:ILE:HG12	2.08	0.53
1:B:126:LYS:NZ	1:B:166:GLU:HB2	2.24	0.53
1:A:380:GLU:HA	1:A:386:TYR:CE2	2.44	0.53
1:A:384:ILE:O	1:A:388:VAL:HG23	2.08	0.53
1:A:698:ASP:HB2	1:A:703:TRP:HZ3	1.73	0.53
1:B:52:TRP:O	1:B:82:VAL:HG23	2.09	0.53
1:A:365:GLN:OE1	1:A:732:MSE:HG2	2.09	0.53
1:B:478:MSE:O	1:B:517:VAL:HG23	2.08	0.52
1:B:612:THR:O	1:B:625:ARG:NH2	2.42	0.52
1:A:462:MSE:HG2	1:A:467:TRP:CZ2	2.44	0.52
1:A:533:THR:HB	1:A:612:THR:CG2	2.39	0.52
1:A:600:TYR:O	1:A:601:ILE:HD12	2.09	0.52
1:A:297:THR:O	1:A:300:LEU:HD13	2.09	0.52
1:B:365:GLN:HE22	1:B:732:MSE:HG2	1.74	0.52
1:A:601:ILE:HD11	1:B:259:LYS:CE	2.31	0.52
1:B:89:VAL:HG13	1:B:93:PHE:HD2	1.75	0.52
1:A:702:VAL:O	1:A:732:MSE:HE3	2.10	0.52
1:B:544:ILE:HB	1:B:640:MSE:HE2	1.90	0.52
1:A:111:ASP:HB3	1:A:158:LEU:CD2	2.40	0.52
1:A:420:ILE:HD12	2:A:743:SAH:HN2	1.75	0.51
1:A:48:ILE:CG2	1:A:326:ARG:HG2	2.40	0.51
1:A:527:SER:HB3	1:A:616:PRO:HD3	1.92	0.51
1:B:169:ARG:HD3	3:B:748:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:HIS:HB2	3:B:775:HOH:O	2.10	0.51
1:B:220:TRP:CD1	1:B:258:TRP:HZ3	2.27	0.51
1:B:407:THR:N	1:B:442:LEU:HD12	2.25	0.51
1:B:411:TYR:HD2	1:B:493:PRO:HB3	1.74	0.51
1:B:63:LEU:HD11	1:B:70:PHE:HD1	1.74	0.51
1:A:478:MSE:C	1:A:480:SER:H	2.14	0.51
1:A:70:PHE:O	1:A:74:LEU:HG	2.10	0.51
1:B:365:GLN:NE2	1:B:732:MSE:HG2	2.25	0.51
1:B:446:LEU:O	1:B:471:VAL:HG23	2.10	0.51
1:B:582:GLN:HG3	1:B:586:ARG:HG2	1.92	0.51
1:A:295:TRP:CH2	1:A:300:LEU:O	2.63	0.51
1:B:207:ASP:C	1:B:209:PHE:H	2.13	0.51
1:A:253:LYS:O	1:B:635:ARG:NE	2.37	0.51
1:A:657:SER:HB3	1:A:662:THR:O	2.10	0.51
1:B:510:SER:N	1:B:511:PRO:CD	2.74	0.51
1:B:648:LEU:O	1:B:655:MSE:HB2	2.11	0.51
1:A:453:PRO:O	1:A:456:ILE:HB	2.10	0.51
1:A:65:ARG:HH11	1:A:461:TYR:HD1	1.59	0.51
1:B:245:LEU:HD13	1:B:287:HIS:CD2	2.46	0.51
1:B:501:LEU:HD22	1:B:648:LEU:HD13	1.93	0.51
1:B:511:PRO:CG	1:B:532:TYR:OH	2.55	0.51
1:B:57:LEU:HD12	1:B:306:ALA:CB	2.29	0.51
1:A:304:LEU:HG	1:A:305:ARG:N	2.26	0.51
1:A:310:THR:OG1	1:A:312:LYS:HA	2.11	0.51
1:A:391:GLU:O	1:A:394:VAL:HG22	2.11	0.51
1:A:695:ARG:HG3	1:A:704:TYR:CE2	2.46	0.51
1:A:388:VAL:HG21	1:A:656:LEU:HD23	1.92	0.51
1:A:691:LEU:HG	1:A:693:ILE:HD11	1.92	0.51
1:A:451:LYS:HG3	1:A:452:ASN:H	1.76	0.50
1:B:112:VAL:HG23	1:B:458:THR:HG23	1.92	0.50
1:B:420:ILE:HD11	1:B:497:VAL:HG12	1.92	0.50
1:A:711:LYS:HG3	1:A:717:SER:HB2	1.92	0.50
1:B:387:ASP:HA	1:B:423:LYS:NZ	2.27	0.50
1:A:367:LEU:O	1:A:451:LYS:HE2	2.12	0.50
1:A:406:LYS:HB3	1:A:440:GLU:OE1	2.12	0.50
1:B:360:LEU:C	1:B:361:GLN:HG3	2.32	0.50
1:A:59:VAL:HG13	1:A:89:VAL:HG11	1.92	0.50
1:B:388:VAL:HA	1:B:391:GLU:HG2	1.94	0.50
1:A:156:CYS:HG	1:A:182:TRP:HZ2	1.59	0.50
1:A:310:THR:HG23	1:A:312:LYS:HG3	1.92	0.50
1:A:55:THR:HG22	1:A:305:ARG:HE	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:541:SER:OG	1:B:544:ILE:HG12	2.12	0.50
1:B:408:VAL:HG23	1:B:442:LEU:HD11	1.92	0.50
1:A:291:LEU:O	1:A:329:VAL:HG12	2.11	0.50
1:B:531:LYS:NZ	1:B:614:GLU:HB3	2.26	0.50
1:B:611:PHE:CE2	1:B:695:ARG:HB2	2.47	0.50
1:A:248:GLU:HA	1:A:254:LEU:HD12	1.93	0.50
1:B:418:GLY:N	1:B:419:PRO:CD	2.75	0.50
1:B:593:TYR:O	1:B:673:ALA:HA	2.12	0.50
1:A:291:LEU:O	1:A:295:TRP:HB2	2.12	0.49
1:B:474:ILE:HD11	1:B:484:ILE:CD1	2.42	0.49
1:B:420:ILE:HD11	1:B:497:VAL:CG1	2.41	0.49
1:B:390:GLY:O	1:B:394:VAL:HG13	2.12	0.49
1:A:541:SER:HB2	1:A:600:TYR:HA	1.94	0.49
1:B:474:ILE:HD11	1:B:484:ILE:HD11	1.94	0.49
1:B:484:ILE:HG13	1:B:484:ILE:O	2.11	0.49
1:B:55:THR:HG22	1:B:56:THR:N	2.27	0.49
1:A:127:ILE:HD12	1:A:127:ILE:N	2.27	0.49
1:A:272:LEU:CD2	1:A:283:ILE:HG23	2.43	0.49
1:B:646:PHE:CE2	1:B:658:ILE:HB	2.47	0.49
1:B:529:PRO:HB3	1:B:650:LEU:HD23	1.94	0.49
1:A:297:THR:HG23	1:A:300:LEU:HD11	1.94	0.49
1:A:315:THR:HG22	1:A:315:THR:O	2.12	0.49
1:A:116:ASN:HD21	1:A:417:ARG:HH12	1.60	0.49
1:A:395:GLY:HA2	1:A:398:LYS:HE2	1.95	0.49
1:B:236:GLN:CB	1:B:264:ALA:HB2	2.42	0.49
1:A:454:ASN:O	1:A:457:VAL:HB	2.13	0.49
1:B:720:THR:HB	1:B:721:PRO:HD2	1.94	0.49
1:B:217:TRP:HA	1:B:258:TRP:CH2	2.47	0.48
1:B:231:SER:HB2	1:B:556:LEU:HD11	1.94	0.48
1:A:571:ASP:C	1:A:571:ASP:OD1	2.51	0.48
1:A:86:ILE:HG21	1:A:155:ILE:HD13	1.95	0.48
1:A:492:GLN:HG2	1:A:520:PHE:O	2.13	0.48
1:A:600:TYR:HD2	1:A:600:TYR:H	1.62	0.48
1:B:615:HIS:HA	1:B:616:PRO:C	2.34	0.48
1:B:592:ILE:HD12	1:B:675:ILE:HG13	1.93	0.48
1:A:400:LEU:CD2	1:A:405:ARG:HH11	2.25	0.48
1:A:277:ARG:HG3	1:A:280:GLU:HG3	1.95	0.48
1:B:405:ARG:HB2	1:B:405:ARG:NH2	2.27	0.48
1:B:698:ASP:HB2	1:B:703:TRP:CZ3	2.40	0.48
1:A:300:LEU:H	1:A:300:LEU:CD1	2.23	0.48
1:A:603:LEU:HB3	1:A:633:MSE:SE	2.63	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:ASN:OD1	1:A:714:ASN:N	2.38	0.48
1:B:162:THR:HG22	1:B:163:MSE:N	2.28	0.48
1:A:165:ILE:HG23	1:A:165:ILE:O	2.14	0.48
1:A:533:THR:HG23	1:A:535:TYR:HE2	1.78	0.48
1:A:283:ILE:HG22	1:A:287:HIS:HB2	1.96	0.48
1:A:176:ALA:HB1	1:A:226:ASN:HB3	1.96	0.48
1:A:310:THR:O	1:A:312:LYS:HG3	2.14	0.48
1:A:608:LYS:HD2	1:A:629:ILE:CG2	2.43	0.48
1:A:649:GLN:HG3	1:A:649:GLN:O	2.14	0.48
1:B:675:ILE:HD12	1:B:675:ILE:N	2.29	0.48
1:A:556:LEU:HA	1:A:556:LEU:HD12	1.65	0.47
1:B:271:GLY:O	1:B:272:LEU:HD13	2.13	0.47
1:B:380:GLU:OE2	1:B:417:ARG:HB2	2.13	0.47
1:B:360:LEU:O	1:B:361:GLN:HG3	2.13	0.47
1:B:607:THR:CG2	1:B:660:PRO:HG2	2.44	0.47
1:B:482:PRO:HB3	1:B:520:PHE:HB3	1.96	0.47
1:A:51:GLY:HA3	1:A:81:PHE:CE1	2.49	0.47
1:A:305:ARG:NH1	1:A:305:ARG:HG2	2.29	0.47
1:B:207:ASP:O	1:B:211:ILE:HG23	2.13	0.47
1:B:531:LYS:HZ1	1:B:614:GLU:HB3	1.79	0.47
1:B:52:TRP:CD1	1:B:74:LEU:HD13	2.50	0.47
1:A:481:LEU:N	1:A:482:PRO:CD	2.78	0.47
1:B:585:VAL:O	1:B:589:MSE:HG2	2.14	0.47
1:B:180:LYS:O	1:B:184:TRP:HD1	1.98	0.47
1:B:486:LYS:HD3	1:B:486:LYS:HA	1.68	0.47
1:A:274:ILE:HD13	1:A:274:ILE:N	2.29	0.47
1:A:590:ASP:HB2	1:A:729:SER:HB2	1.97	0.47
1:A:67:VAL:HG21	1:A:109:LEU:HD11	1.96	0.47
1:A:191:THR:HG22	1:A:192:VAL:N	2.30	0.47
1:A:317:ILE:HG13	1:A:320:GLU:CD	2.34	0.47
1:A:420:ILE:O	1:A:424:ILE:HG13	2.14	0.47
1:A:55:THR:CG2	1:A:305:ARG:HE	2.27	0.47
1:A:648:LEU:O	1:A:655:MSE:HB2	2.14	0.47
1:A:648:LEU:HD23	1:A:656:LEU:HD12	1.96	0.47
1:A:697:VAL:HG13	1:A:702:VAL:HG22	1.97	0.47
1:A:533:THR:O	1:A:646:PHE:HA	2.15	0.47
1:A:595:VAL:O	1:A:672:PRO:HD2	2.13	0.47
1:A:647:ASP:C	1:A:647:ASP:OD1	2.53	0.47
1:B:383:GLN:HG2	1:B:384:ILE:N	2.29	0.47
1:B:662:THR:O	1:B:662:THR:HG22	2.15	0.47
1:A:517:VAL:O	1:A:517:VAL:HG13	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:ASP:O	1:A:518:THR:HG23	2.15	0.46
1:B:67:VAL:HG21	1:B:109:LEU:HD11	1.96	0.46
1:B:196:LEU:HD11	1:B:220:TRP:HB2	1.97	0.46
1:A:215:ASP:OD2	1:A:257:ARG:NH2	2.49	0.46
1:A:517:VAL:CG1	1:A:521:LEU:HD21	2.44	0.46
1:B:710:LYS:O	1:B:717:SER:HA	2.16	0.46
1:A:295:TRP:CD1	1:A:329:VAL:HB	2.50	0.46
1:A:407:THR:HA	1:A:443:LYS:O	2.14	0.46
1:B:126:LYS:HZ1	1:B:166:GLU:HB2	1.79	0.46
1:B:56:THR:HA	1:B:59:VAL:CG2	2.45	0.46
1:A:186:ARG:HD3	1:A:186:ARG:HA	1.73	0.46
1:A:367:LEU:HD13	2:A:743:SAH:HN61	1.81	0.46
1:A:55:THR:C	1:A:57:LEU:H	2.18	0.46
1:A:690:SER:HB3	1:A:692:LYS:HZ3	1.81	0.46
1:B:162:THR:HG23	1:B:191:THR:HB	1.97	0.46
1:A:386:TYR:CE1	1:A:419:PRO:HB2	2.50	0.46
1:A:539:ILE:CD1	1:A:640:MSE:HE3	2.45	0.46
1:B:44:ALA:HB3	1:B:47:ARG:HD3	1.97	0.46
1:B:451:LYS:O	1:B:453:PRO:HD3	2.16	0.46
1:A:171:SER:C	1:A:173:PRO:HD3	2.35	0.46
1:B:86:ILE:HD11	1:B:151:GLU:CG	2.43	0.46
1:A:308:THR:C	1:A:310:THR:H	2.19	0.46
1:B:90:VAL:O	1:B:105:PRO:HG2	2.16	0.46
1:A:78:LYS:HE2	1:A:326:ARG:HH11	1.80	0.46
1:B:133:CYS:HB2	1:B:175:THR:OG1	2.16	0.46
1:B:215:ASP:H	1:B:218:THR:HB	1.81	0.46
1:A:125:GLY:O	1:A:163:MSE:HG2	2.16	0.46
1:A:277:ARG:HG3	1:A:280:GLU:CG	2.46	0.46
1:A:398:LYS:HD3	1:A:435:PHE:CZ	2.50	0.46
1:A:532:TYR:HB3	1:A:648:LEU:CB	2.40	0.46
1:A:78:LYS:HB3	1:A:78:LYS:NZ	2.30	0.46
1:B:317:ILE:O	1:B:317:ILE:HG22	2.16	0.46
1:A:168:THR:HB	1:A:204:LYS:HZ3	1.80	0.45
1:A:698:ASP:HA	3:A:798:HOH:O	2.16	0.45
1:B:659:GLU:HG3	1:B:660:PRO:HD2	1.97	0.45
1:B:680:GLN:HG3	3:B:783:HOH:O	2.15	0.45
1:A:295:TRP:CZ3	1:A:302:ILE:HG13	2.52	0.45
1:B:155:ILE:HD12	1:B:163:MSE:HG3	1.98	0.45
1:B:272:LEU:HA	1:B:272:LEU:HD12	1.75	0.45
1:B:572:GLU:HG2	1:B:573:ASP:OD1	2.16	0.45
1:A:126:LYS:HA	1:A:164:ALA:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:ASN:OD1	1:A:452:ASN:C	2.55	0.45
1:A:624:GLU:O	1:A:625:ARG:HD3	2.17	0.45
1:A:193:TRP:CH2	1:A:301:ARG:HD3	2.52	0.45
1:A:527:SER:HB2	1:A:616:PRO:HG3	1.98	0.45
1:A:648:LEU:CD2	1:A:656:LEU:HD12	2.46	0.45
1:B:538:PRO:HD3	1:B:631:PHE:CE1	2.52	0.45
1:A:727:GLY:O	1:A:731:TYR:HB2	2.17	0.45
1:B:533:THR:CG2	1:B:612:THR:HG22	2.46	0.45
1:B:689:ILE:HD13	1:B:710:LYS:HA	1.99	0.45
1:A:703:TRP:HA	1:A:732:MSE:CE	2.46	0.45
1:B:608:LYS:HB3	1:B:609:PRO:HD2	1.99	0.45
1:B:80:ASN:ND2	1:B:80:ASN:H	2.14	0.45
1:B:249:LEU:C	1:B:255:VAL:HG22	2.38	0.44
1:B:659:GLU:HG3	1:B:660:PRO:CD	2.47	0.44
1:A:295:TRP:CG	1:A:329:VAL:HB	2.52	0.44
1:A:703:TRP:NE1	1:A:705:GLU:HG3	2.31	0.44
1:B:163:MSE:SE	1:B:192:VAL:HG22	2.68	0.44
1:A:50:ILE:HD13	1:A:302:ILE:HB	1.99	0.44
1:A:537:LYS:HA	1:A:538:PRO:HD3	1.88	0.44
1:B:692:LYS:O	1:B:706:TRP:HA	2.17	0.44
1:A:272:LEU:HD21	1:A:283:ILE:HG23	2.00	0.44
1:A:315:THR:HG23	1:A:318:LYS:HE3	2.00	0.44
1:A:383:GLN:NE2	1:A:383:GLN:H	2.15	0.44
1:A:527:SER:HB3	1:A:616:PRO:CD	2.48	0.44
1:A:636:ASN:HA	1:A:684:GLY:HA2	2.00	0.44
1:B:509:LEU:HD11	1:B:702:VAL:HB	1.99	0.44
1:B:529:PRO:HA	1:B:650:LEU:HA	1.99	0.44
1:B:326:ARG:C	1:B:328:ALA:N	2.71	0.44
1:B:53:MSE:HG3	1:B:83:VAL:HB	2.00	0.44
1:A:287:HIS:HE1	3:A:779:HOH:O	2.01	0.43
1:B:383:GLN:NE2	1:B:383:GLN:H	2.16	0.43
1:B:495:ILE:HG23	1:B:526:ILE:HD11	2.01	0.43
1:B:520:PHE:C	1:B:520:PHE:CD2	2.91	0.43
1:B:537:LYS:HA	1:B:538:PRO:HD3	1.87	0.43
1:A:207:ASP:C	1:A:209:PHE:H	2.21	0.43
1:A:290:LEU:HD23	1:A:291:LEU:HD12	2.00	0.43
1:B:501:LEU:N	1:B:501:LEU:HD12	2.33	0.43
1:A:86:ILE:CD1	1:A:151:GLU:HB3	2.48	0.43
1:A:411:TYR:CD1	1:A:447:TYR:HB2	2.54	0.43
1:A:456:ILE:HG13	1:A:475:GLU:HG3	2.00	0.43
1:B:253:LYS:HE2	1:B:253:LYS:HB3	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:443:LYS:HE3	1:B:470:ARG:NH2	2.33	0.43
1:B:703:TRP:HA	1:B:732:MSE:HE2	1.99	0.43
1:A:590:ASP:HB2	1:A:729:SER:CB	2.48	0.43
1:B:207:ASP:O	1:B:209:PHE:N	2.51	0.43
1:B:413:LEU:HB3	1:B:478:MSE:SE	2.67	0.43
1:A:103:HIS:HA	1:A:104:PRO:HD3	1.87	0.43
1:A:145:GLU:OE2	1:A:174:ARG:NH2	2.50	0.43
1:A:196:LEU:HD21	1:A:220:TRP:HB2	1.99	0.43
1:A:628:SER:C	1:A:629:ILE:HD13	2.39	0.43
1:A:633:MSE:HG2	1:A:683:VAL:CG2	2.48	0.43
1:A:509:LEU:CD2	1:A:509:LEU:N	2.82	0.43
1:B:89:VAL:HG22	1:B:93:PHE:HE2	1.84	0.43
1:B:198:SER:HB2	1:B:202:LYS:CD	2.39	0.43
1:B:206:TYR:CE2	1:B:211:ILE:HD13	2.53	0.43
1:B:211:ILE:O	1:B:211:ILE:HG13	2.18	0.43
1:B:251:GLU:O	1:B:255:VAL:HG23	2.19	0.43
1:B:481:LEU:N	1:B:482:PRO:CD	2.81	0.43
1:B:697:VAL:HG12	1:B:698:ASP:N	2.34	0.43
1:A:209:PHE:O	1:A:209:PHE:CG	2.72	0.43
1:A:134:ASP:HA	3:A:776:HOH:O	2.19	0.42
1:B:122:TYR:CD1	1:B:122:TYR:N	2.84	0.42
1:B:288:ILE:HG23	1:B:292:LYS:HE3	2.01	0.42
1:B:630:GLU:C	1:B:631:PHE:CD2	2.93	0.42
1:A:148:LEU:HD23	1:A:178:ILE:HG21	2.01	0.42
1:A:616:PRO:HG2	1:A:618:PHE:CZ	2.54	0.42
1:A:709:GLU:HG2	1:A:719:SER:HB2	2.01	0.42
1:B:294:LEU:HD23	1:B:294:LEU:HA	1.82	0.42
1:B:112:VAL:HG11	1:B:462:MSE:HE1	2.01	0.42
1:B:485:ALA:O	1:B:490:PHE:N	2.52	0.42
1:B:569:GLU:OE1	1:B:579:LYS:HE2	2.19	0.42
1:A:154:TYR:HD1	1:A:454:ASN:OD1	2.03	0.42
1:A:47:ARG:HD3	1:A:48:ILE:H	1.84	0.42
1:A:559:ALA:HB2	1:A:576:TRP:O	2.19	0.42
1:B:91:ARG:HA	1:B:105:PRO:HG2	2.00	0.42
1:A:232:GLY:O	1:A:236:GLN:HG2	2.20	0.42
1:A:459:LEU:HB3	1:A:473:ILE:HD12	2.01	0.42
1:A:585:VAL:O	1:A:588:ASN:HB2	2.19	0.42
1:B:311:PHE:CD2	1:B:312:LYS:HD2	2.54	0.42
1:B:425:LEU:HA	1:B:428:GLU:HG2	2.02	0.42
1:A:128:SER:HB3	1:A:130:TRP:NE1	2.34	0.42
1:A:253:LYS:HB3	1:A:253:LYS:HE2	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ARG:HH21	1:A:405:ARG:HG2	1.85	0.42
1:A:380:GLU:OE2	1:A:417:ARG:HD3	2.20	0.42
1:B:115:ARG:HG2	1:B:118:LEU:HG	2.00	0.42
1:B:273:PHE:CD1	1:B:273:PHE:N	2.88	0.42
1:B:249:LEU:HB3	1:B:290:LEU:CD1	2.49	0.42
1:A:47:ARG:HD2	1:A:47:ARG:N	2.33	0.42
1:B:724:ASN:OD1	1:B:727:GLY:HA2	2.19	0.42
1:A:454:ASN:ND2	1:A:454:ASN:H	2.18	0.42
1:A:497:VAL:HA	1:A:528:ILE:O	2.20	0.42
1:A:601:ILE:CD1	1:B:259:LYS:HB2	2.50	0.42
1:A:640:MSE:C	1:A:640:MSE:SE	3.09	0.42
1:A:216:LEU:O	1:A:219:ILE:HB	2.20	0.41
1:B:110:PRO:HG2	1:B:461:TYR:CD1	2.55	0.41
1:B:646:PHE:H	1:B:658:ILE:HG22	1.85	0.41
1:A:111:ASP:N	1:A:111:ASP:OD1	2.54	0.41
1:A:385:LYS:HB3	1:A:385:LYS:HE2	1.91	0.41
1:B:165:ILE:O	1:B:165:ILE:HG23	2.20	0.41
1:B:171:SER:C	1:B:173:PRO:HD3	2.40	0.41
1:B:212:GLU:HG3	3:B:775:HOH:O	2.20	0.41
1:A:300:LEU:N	1:A:300:LEU:HD12	2.29	0.41
1:A:74:LEU:HD22	1:A:79:TYR:OH	2.20	0.41
1:B:110:PRO:O	1:B:113:GLN:HG2	2.20	0.41
1:B:295:TRP:HZ3	1:B:302:ILE:HG13	1.85	0.41
1:B:514:LEU:HA	1:B:514:LEU:HD23	1.89	0.41
1:B:613:PHE:CD1	1:B:625:ARG:NH1	2.89	0.41
1:B:697:VAL:HG22	1:B:702:VAL:HG22	2.02	0.41
1:A:486:LYS:HB3	1:A:486:LYS:NZ	2.36	0.41
1:B:532:TYR:CE2	1:B:615:HIS:CE1	3.09	0.41
1:A:220:TRP:CZ3	1:A:237:VAL:HB	2.55	0.41
1:A:283:ILE:HG22	1:A:287:HIS:HB3	2.00	0.41
1:A:314:ASN:O	1:A:315:THR:CB	2.69	0.41
1:A:277:ARG:CB	1:A:280:GLU:HG2	2.38	0.41
1:B:411:TYR:HB2	1:B:496:ILE:HG22	2.02	0.41
1:B:532:TYR:CE2	1:B:615:HIS:HE1	2.39	0.41
1:B:454:ASN:N	1:B:454:ASN:HD22	2.18	0.41
1:A:128:SER:HA	1:A:129:PRO:HD3	1.87	0.41
1:A:124:VAL:HG22	1:A:162:THR:HB	2.02	0.41
1:B:379:PHE:HD1	1:B:379:PHE:HA	1.72	0.41
1:B:380:GLU:HA	1:B:386:TYR:OH	2.21	0.41
1:A:116:ASN:HD21	1:A:417:ARG:NH1	2.19	0.41
1:A:200:ILE:H	1:A:200:ILE:HG13	1.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:PHE:CE1	1:A:315:THR:O	2.74	0.41
1:A:481:LEU:N	1:A:482:PRO:HD2	2.36	0.41
1:A:498:SER:CB	1:A:514:LEU:HD21	2.51	0.41
1:A:682:ARG:HH21	1:B:221:ALA:CB	2.31	0.41
1:B:172:SER:N	1:B:173:PRO:HD3	2.36	0.41
1:B:410:ILE:HD13	1:B:444:VAL:HG13	2.02	0.41
1:B:658:ILE:O	1:B:658:ILE:HD13	2.21	0.41
1:A:312:LYS:C	1:A:314:ASN:H	2.25	0.41
1:A:418:GLY:N	1:A:419:PRO:CD	2.84	0.41
1:A:697:VAL:HG12	1:A:698:ASP:N	2.36	0.41
1:B:689:ILE:HD13	1:B:689:ILE:HA	1.83	0.41
1:A:406:LYS:N	1:A:406:LYS:CD	2.83	0.40
1:A:431:TYR:CE2	1:A:442:LEU:HD23	2.56	0.40
1:A:493:PRO:HD3	1:A:520:PHE:CE2	2.56	0.40
1:A:677:LEU:HA	1:A:723:GLN:OE1	2.21	0.40
1:A:709:GLU:HG2	1:A:719:SER:CB	2.51	0.40
1:B:114:LEU:HG	1:B:118:LEU:HD12	2.03	0.40
1:B:640:MSE:SE	1:B:640:MSE:C	3.10	0.40
1:A:180:LYS:O	1:A:183:ILE:HG13	2.20	0.40
1:A:274:ILE:O	1:A:279:GLY:HA2	2.21	0.40
1:A:79:TYR:HD1	1:A:79:TYR:O	2.04	0.40
1:B:506:ASP:OD1	1:B:695:ARG:NE	2.37	0.40
1:B:528:ILE:HA	1:B:529:PRO:HA	1.92	0.40
1:A:410:ILE:HD12	1:A:444:VAL:HG11	2.04	0.40
1:A:412:LEU:HB3	1:A:448:ILE:HG12	2.03	0.40
1:A:154:TYR:CD1	1:A:454:ASN:OD1	2.74	0.40
1:B:383:GLN:HG2	1:B:384:ILE:HG13	2.04	0.40
1:B:509:LEU:CD2	1:B:732:MSE:HB3	2.50	0.40
1:A:422:THR:HG22	1:A:467:TRP:NE1	2.16	0.40
1:A:724:ASN:OD1	1:A:727:GLY:HA2	2.22	0.40
1:B:569:GLU:CD	1:B:579:LYS:HE2	2.42	0.40
1:A:591:GLN:HB2	1:A:593:TYR:CE1	2.56	0.40
1:A:67:VAL:HG12	1:A:71:CYS:SG	2.62	0.40
1:B:115:ARG:CG	1:B:118:LEU:HG	2.51	0.40
1:B:263:LEU:HD12	1:B:264:ALA:N	2.36	0.40
1:B:314:ASN:O	1:B:315:THR:C	2.58	0.40
1:B:536:VAL:HG11	1:B:691:LEU:HD23	2.03	0.40
1:B:629:ILE:HD13	1:B:629:ILE:N	2.36	0.40
1:B:664:THR:HB	1:B:667:MSE:SE	2.72	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	658/745 (88%)	579 (88%)	72 (11%)	7 (1%)	14 50
1	B	643/745 (86%)	581 (90%)	56 (9%)	6 (1%)	17 55
All	All	1301/1490 (87%)	1160 (89%)	128 (10%)	13 (1%)	15 53

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	312	LYS
1	A	97	ASN
1	A	182	TRP
1	A	315	THR
1	B	212	GLU
1	A	309	ASP
1	A	271	GLY
1	B	208	ALA
1	B	327	HIS
1	A	479	ARG
1	B	211	ILE
1	B	452	ASN
1	B	484	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	587/645 (91%)	527 (90%)	60 (10%)	7 28

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	577/645 (90%)	515 (89%)	62 (11%)	6 26
All	All	1164/1290 (90%)	1042 (90%)	122 (10%)	7 27

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ASN
1	A	47	ARG
1	A	55	THR
1	A	58	ASP
1	A	80	ASN
1	A	86	ILE
1	A	101	GLU
1	A	108	ASP
1	A	155	ILE
1	A	180	LYS
1	A	186	ARG
1	A	187	ASN
1	A	190	PHE
1	A	201	GLU
1	A	213	HIS
1	A	257	ARG
1	A	274	ILE
1	A	278	ASN
1	A	283	ILE
1	A	290	LEU
1	A	297	THR
1	A	304	LEU
1	A	311	PHE
1	A	316	SER
1	A	319	SER
1	A	368	SER
1	A	383	GLN
1	A	399	ASP
1	A	406	LYS
1	A	433	ASN
1	A	462	MSE
1	A	471	VAL
1	A	499	GLU
1	A	504	PHE
1	A	517	VAL
1	A	520	PHE

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Mol	Chain	Res	Type
1	A	521	LEU
1	A	526	ILE
1	A	528	ILE
1	A	533	THR
1	A	536	VAL
1	A	547	THR
1	A	558	ARG
1	A	575	MSE
1	A	586	ARG
1	A	595	VAL
1	A	600	TYR
1	A	601	ILE
1	A	612	THR
1	A	614	GLU
1	A	627	ASP
1	A	635	ARG
1	A	640	MSE
1	A	648	LEU
1	A	653	THR
1	A	658	ILE
1	A	687	ASP
1	A	694	ASP
1	A	713	THR
1	A	734	MSE
1	B	56	THR
1	B	80	ASN
1	B	82	VAL
1	B	101	GLU
1	B	102	ASN
1	B	108	ASP
1	B	117	ASP
1	B	151	GLU
1	B	163	MSE
1	B	186	ARG
1	B	187	ASN
1	B	191	THR
1	B	200	ILE
1	B	201	GLU
1	B	257	ARG
1	B	263	LEU
1	B	272	LEU
1	B	290	LEU

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Mol	Chain	Res	Type
1	B	300	LEU
1	B	305	ARG
1	B	309	ASP
1	B	312	LYS
1	B	321	TYR
1	B	327	HIS
1	B	360	LEU
1	B	361	GLN
1	B	378	THR
1	B	379	PHE
1	B	383	GLN
1	B	405	ARG
1	B	406	LYS
1	B	409	VAL
1	B	428	GLU
1	B	429	ARG
1	B	468	LYS
1	B	472	THR
1	B	474	ILE
1	B	486	LYS
1	B	487	ASP
1	B	509	LEU
1	B	510	SER
1	B	513	CYS
1	B	520	PHE
1	B	594	VAL
1	B	596	TYR
1	B	600	TYR
1	B	614	GLU
1	B	632	VAL
1	B	635	ARG
1	B	640	MSE
1	B	648	LEU
1	B	649	GLN
1	B	652	LYS
1	B	656	LEU
1	B	658	ILE
1	B	659	GLU
1	B	663	HIS
1	B	693	ILE
1	B	707	HIS
1	B	713	THR

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Mol	Chain	Res	Type
1	B	714	ASN
1	B	733	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	327	HIS
1	A	454	ASN
1	A	551	GLN
1	A	563	HIS
1	A	649	GLN
1	B	116	ASN
1	B	195	GLN
1	B	377	ASN
1	B	383	GLN
1	B	454	ASN
1	B	551	GLN
1	B	615	HIS
1	B	649	GLN
1	B	707	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SAH	A	743	-	21,28,28	1.15	2 (9%)	20,40,40	1.78	3 (15%)
2	SAH	B	743	-	21,28,28	1.19	2 (9%)	20,40,40	1.74	3 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	A	743	-	-	1/7/31/31	0/3/3/3
2	SAH	B	743	-	-	3/7/31/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	743	SAH	C2-N3	3.84	1.38	1.32
2	A	743	SAH	C2-N3	3.75	1.38	1.32
2	A	743	SAH	C2-N1	2.47	1.38	1.33
2	B	743	SAH	C2-N1	2.45	1.38	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	743	SAH	N3-C2-N1	-5.52	120.06	128.68
2	B	743	SAH	N3-C2-N1	-5.37	120.28	128.68
2	A	743	SAH	C5'-SD-CG	-4.24	89.53	102.27
2	B	743	SAH	C5'-SD-CG	-3.54	91.65	102.27
2	B	743	SAH	C3'-C2'-C1'	2.80	105.20	100.98
2	A	743	SAH	C3'-C2'-C1'	2.05	104.07	100.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	743	SAH	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
2	B	743	SAH	N-CA-CB-CG
2	B	743	SAH	CB-CG-SD-C5'
2	A	743	SAH	CB-CG-SD-C5'

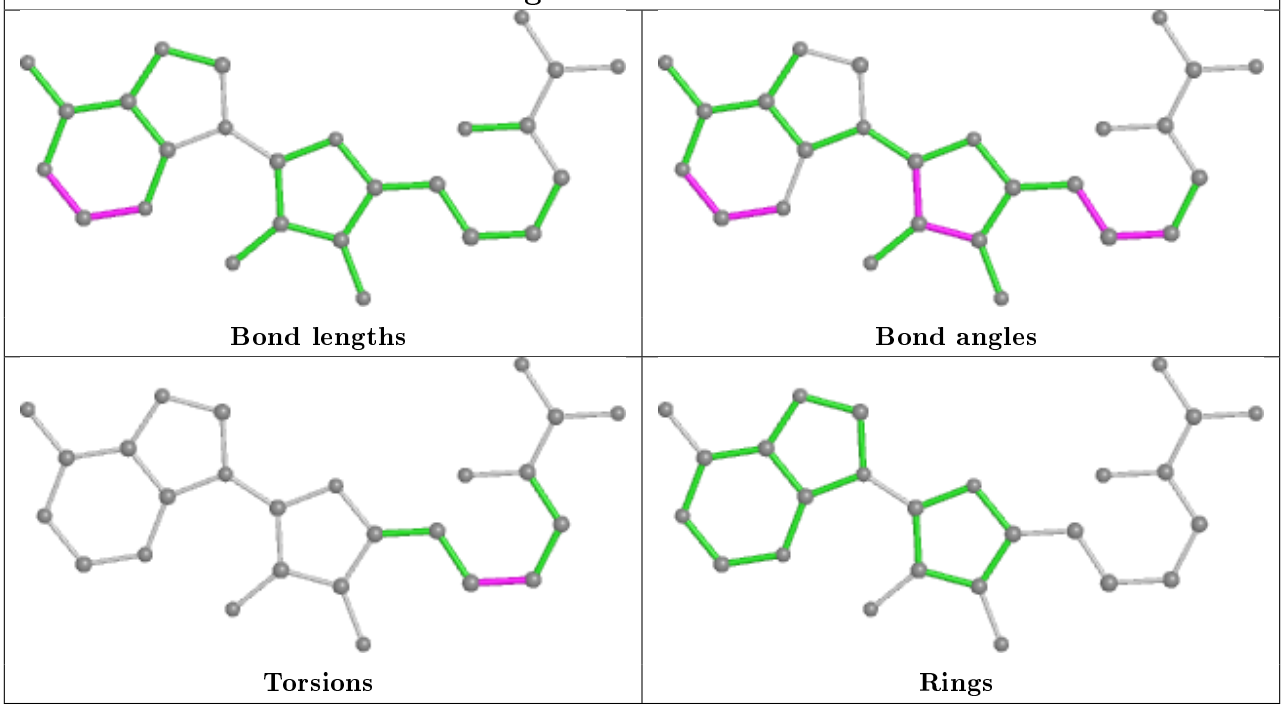
There are no ring outliers.

1 monomer is involved in 3 short contacts:

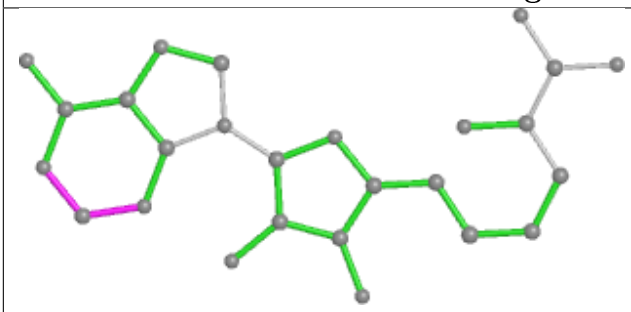
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	743	SAH	3	0

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

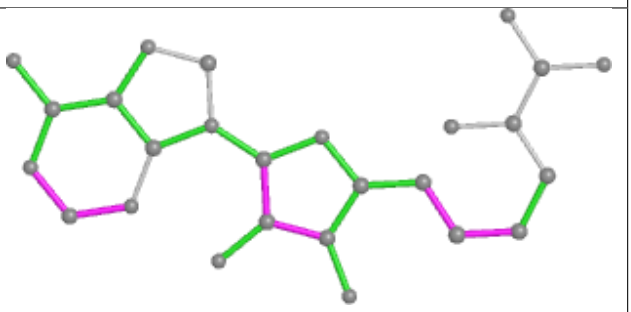
Ligand SAH A 743



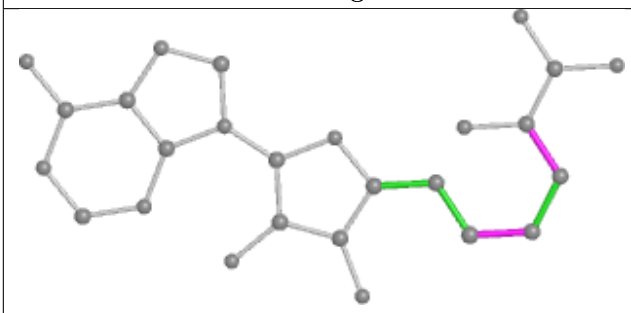
Ligand SAH B 743



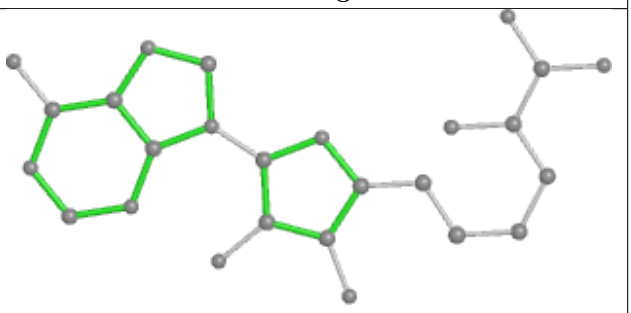
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	648/745 (86%)	-0.42	8 (1%) 79 54	12, 78, 146, 239	0
1	B	637/745 (85%)	-0.24	6 (0%) 84 63	16, 88, 162, 216	13 (2%)
All	All	1285/1490 (86%)	-0.33	14 (1%) 80 56	12, 82, 154, 239	13 (1%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	313	TYR	4.9
1	B	429	ARG	3.7
1	B	308	THR	3.5
1	A	313	TYR	3.3
1	A	311	PHE	2.7
1	A	99	SER	2.6
1	B	406	LYS	2.6
1	B	287	HIS	2.3
1	B	316	SER	2.3
1	A	327	HIS	2.3
1	A	314	ASN	2.2
1	A	713	THR	2.2
1	A	490	PHE	2.2
1	A	275	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands (i)

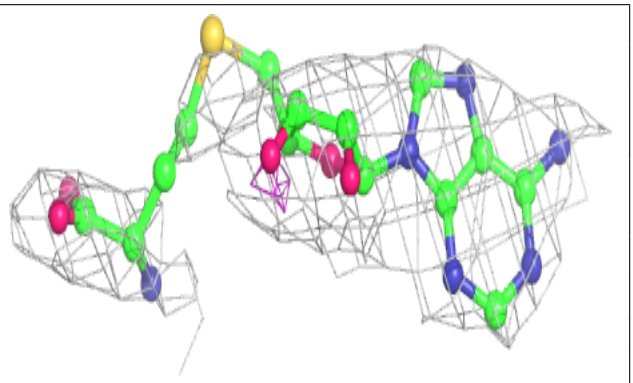
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

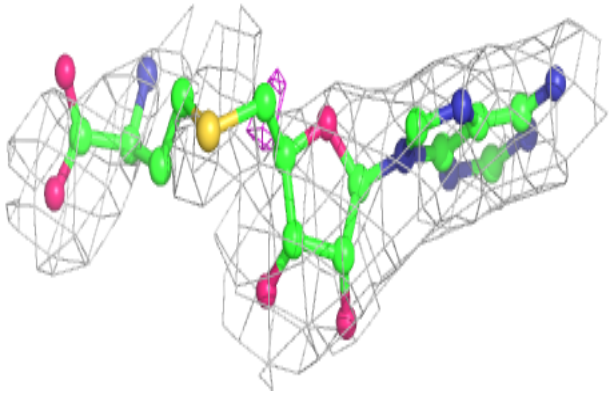
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SAH	B	743	26/26	0.93	0.20	85,97,121,203	0
2	SAH	A	743	26/26	0.96	0.14	70,75,88,99	0

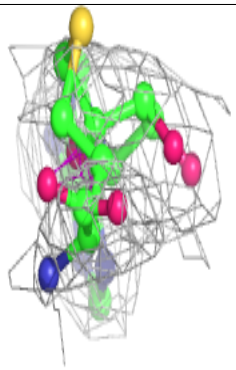
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAH B 743:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

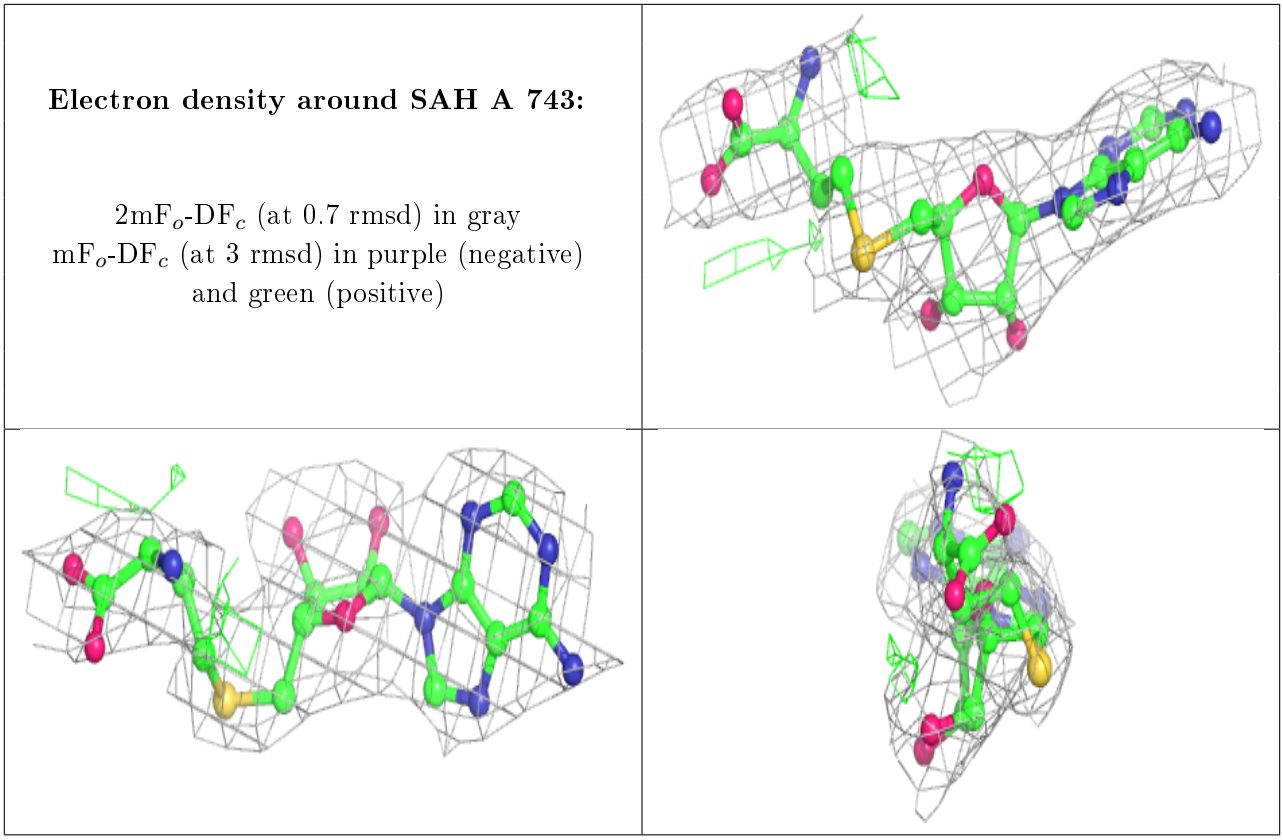






Electron density around SAH A 743:

$2mF_o$-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.