



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:36 PM GMT

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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

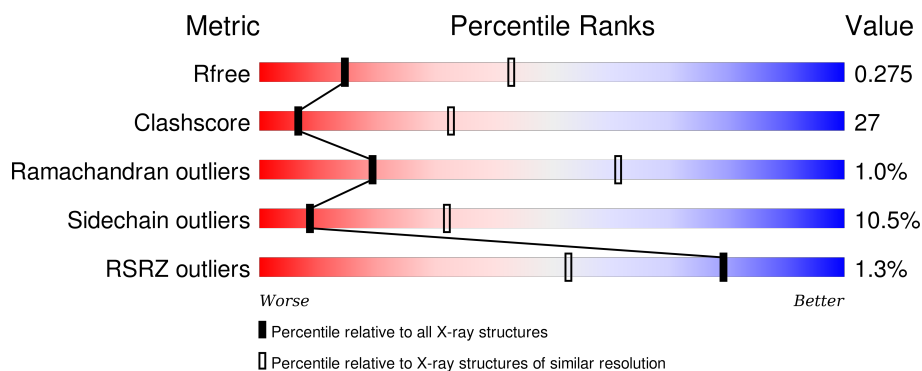
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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. 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	745	<div> <div></div> <div> <div></div> <div>47%</div> <div>37%</div> <div>5%</div> <div>11%</div> </div> </div>
1	B	745	<div> <div></div> <div> <div></div> <div>47%</div> <div>35%</div> <div>6%</div> <div>13%</div> </div> </div>

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: C₁₄H₂₀N₆O₅S).



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		

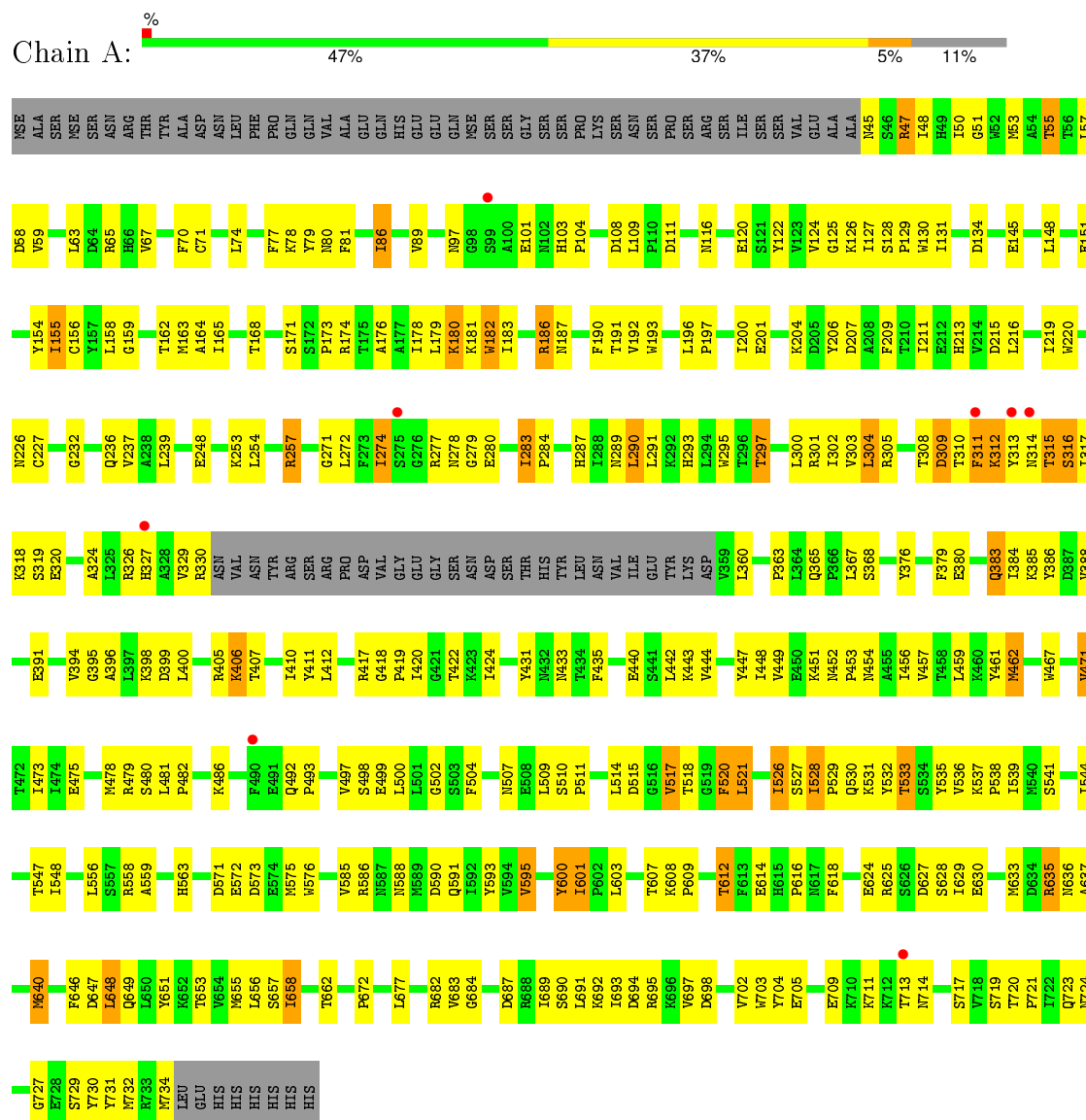
- Molecule 3 is water.

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

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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



6727	Q649	T547	I473	V393	K318	L249	R169	V67	WSE
L650	L650	L556	I474	V394	Y321	T250	I170	A68	ALA
T651	T651	L556	I474	V394	Y321	E251	S171	T69	SER
T652	T652	L556	I474	V394	Y321	L252	S172	F70	SER
T653	T653	S562	L481	R405	R326	K253	P173	R73	ASN
T654	T654	E569	P482	T407	H327	L254	H174	L74	ARG
T655	T655	E569	P482	V408	A328	V255	T175		THR
T656	T656	E572	P483	V409	VAL	D256			TYR
T657	T657	D573	I484	Y411	ARG	K257			ALA
T658	T658	D573	A485	Y412	ASN	W258	K180	F77	ASP
T659	T659	K486	K486	L412	VAL	K259	K181	F78	ASN
T660	T660	D487	D487	L413	ASN		Y79	Y79	LEU
T661	T661				TYR	L263	H184		
T662	T662	K579	P480	R417	ARG	A264	T185	F81	PHE
T663	T663	Q582	E491	G418	SER	A265	R186	W82	PRO
T664	T664	Q582	Q492	P419	ARG	F266	N187	V83	GLN
T665	T665	P493	P493	I420	PRO	V267	S188		GLN
T666	T666	V585	P494	G421	ASP	S189	S188	I86	VAL
T667	T667	R586	I495	T422	VAL	G271	F190	G87	ALA
T668	T668	M589	I496	K423	GLY	L272	T191	G88	GLU
T669	T669	M589	I497	I424	GLY	F273	V192	W89	GLN
T670	T670	I592	L500	L425	GLY	I1E	L196	V90	HIS
T671	T671	Y593	L501	E428	ASN		P197	R91	GLU
T672	T672	V594	A502	R429	ASP		S198	A92	GLU
T673	T673	V595	S503	B429	SER		A199	F93	GLN
T674	T674	Y596		R436	THR		I200		WSE
T675	T675	Y596		GLN	HIS		E201	E101	SER
T680	T680	Y600	D506	GLN	TYR		K202	M102	GLY
T688	T688	I601	L509	GLN	LEU		Y206	P104	SER
T689	T689	P602	S510	GLU	ASN		D207	P105	SER
T690	T690	T607	E512	S441	VAL		A208		PRO
T691	T691	K608	C513	L442	ILE		F209	D108	LYS
T693	T693	P609	L514	K443	GLU		T210	L109	SER
T694	T694	V610	V517	K445	TYR		D111	P110	ASN
T695	T695	F611	V517	K446	LYS		E212	D111	SER
T696	T696	T612	T518	L446	ASP		H213	V112	PRO
T697	T697	F613	G519	V449	V359		D215	Q113	SER
T698	T698	E614	P520	E450	L360		W214	L114	ARG
T702	T702	H615	L521	K451	Q361		D216	R115	SER
T703	T703	P616	K522	N452	Q365		W217	N116	ILE
T706	T706	E624	I526	P453	Y375		T218	D117	SER
T707	T707	I629	S527	N454			I219	L118	SER
T710	T710	E630	P529	T458	T378		W220	Y122	VAL
T711	T711	F631	Q530	L459	F379		A221		GLU
T712	T712	V632	K531	K460	E380		K126		A43
T713	T713	V632	Y532	Y461	E381		C227		A44
T714	T714	R635	T533	M462	D382		S231		B47
T715	T715	M640	V536	M463	Q383		Y234		W52
T716	T716	G641	K537	R465	I384		F235		W53
T717	T717	F642	P538	R466	K385		Q236		A54
T720	T720	F646	S541	K468	D387		T240		T55
T721	T721	D647	I544	R469	V388		L245		T56
T724	T724	L648		R470	Y389		L245		L57
				V471	G390		L245		W58
				T472	E391		L245		W59
					A392		L245		L63

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.38 Å 129.38 Å 149.31 Å 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
$\langle I/\sigma(I) \rangle$ ¹	5.41 (at 3.00 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.223 , 0.281 0.217 , 0.275	Depositor DCC
R_{free} test set	1827 reflections (4.62%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 39562 reflections (0.003%)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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:CE2	1:B:74:LEU:HD11	2.19	0.77
1:B:70:PHE:HE2	1:B:74:LEU:HD11	1.48	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

Continued on next page...

Continued from previous page...

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:537:LYS:HE2	1:B:602:PRO:HB3	1.72	0.71
1:B:215:ASP:HB2	1:B:248:GLU:OE1	1.91	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:536:VAL:HG22	1:B:642:PHE:HB3	1.74	0.69
1:B:449:VAL:HA	1:B:474:ILE:HG23	1.74	0.69
1:B:212:GLU:HG3	1:B:213:HIS:H	1.58	0.69
1:B:59:VAL:HG13	1:B:89:VAL:HG11	1.73	0.69
1:B:509:LEU:HD21	1:B:732:MSE:CB	2.22	0.69
1:B:635:ARG:HG2	1:B:635:ARG:NH1	2.03	0.69
1:B:405:ARG:HH21	1:B:405:ARG:HB2	1.56	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:284:PRO:HG2	1:B:287:HIS:CG	2.27	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:B:600:TYR:O	1:B:601:ILE:HD12	1.95	0.66
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: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

Continued on next page...

Continued from previous page...

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:B:537:LYS:HB2	1:B:607:THR:HG22	1.78	0.65
1:A:497:VAL:HG22	1:A:528:ILE:HG23	1.79	0.65
1:A:179:LEU:O	1:A:183:ILE:HG12	1.97	0.64
1:B:418:GLY:N	1:B:419:PRO:HD3	2.12	0.64
1:A:254:LEU:O	1:A:257:ARG:HD3	1.98	0.64
1:B:70:PHE:O	1:B:74:LEU:HG	1.98	0.64
1:A:86:ILE:HG21	1:A:155:ILE:CD1	2.28	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:B:389:TYR:O	1:B:393:VAL:HG23	1.98	0.63
1:A:400:LEU:HD22	1:A:405:ARG:HE	1.63	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:B:189:ARG:HB3	1:B:234:TYR:CE1	2.32	0.63
1:A:517:VAL:HG13	1:A:521:LEU:HD21	1.81	0.63
1:B:541:SER:HB2	1:B:600:TYR:CB	2.28	0.62
1:B:532:TYR:CE1	1:B:613:PHE:HB2	2.35	0.62
1:A:127:ILE:CG2	1:A:131:ILE:HD12	2.29	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:509:LEU:HD21	1:B:732:MSE:HB3	1.82	0.62
1:B:201:GLU:HA	1:B:206:TYR:CE2	2.34	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:509:LEU:HD21	1:B:732:MSE:HB2	1.82	0.61
1:B:412:LEU:HD21	1:B:420:ILE:HG23	1.83	0.61
1:A:220:TRP:CE3	1:A:237:VAL:HB	2.35	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:ILE:HG21	1:B:155:ILE:HD13	1.81	0.61
1:B:688:ARG:NH1	1:B:711:LYS:HD2	2.15	0.61
1:B:56:THR:HA	1:B:59:VAL:HG23	1.81	0.61
1:A:310:THR:C	1:A:312:LYS:N	2.52	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:635:ARG:HH11	1:B:635:ARG:CG	2.14	0.59
1:B:245:LEU:HD13	1:B:287:HIS:NE2	2.18	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:B:86:ILE:HD13	1:B:155:ILE:CD1	2.34	0.58
1:A:720:THR:HB	1:A:721:PRO:HD2	1.85	0.58
1:B:410:ILE:HG13	1:B:495:ILE:HB	1.86	0.58
1:B:326:ARG:C	1:B:328:ALA:H	2.07	0.58
1:B:536:VAL:HG22	1:B:642:PHE:CB	2.33	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:A:363:PRO:HG2	1:A:730:TYR:OH	2.03	0.58
1:B:624:GLU:O	1:B:625:ARG:HD3	2.04	0.57
1:A:637:ALA:HA	1:B:217:TRP:CH2	2.39	0.57
1:A:500:LEU:O	1:A:510:SER:HB2	2.04	0.57
1:A:418:GLY:N	1:A:419:PRO:HD3	2.19	0.57
1:A:78:LYS:HE2	1:A:326:ARG:NH1	2.19	0.57
1:A:274:ILE:HD13	1:A:274:ILE:H	1.69	0.57
1:A:120:GLU:HG2	1:A:159:GLY:O	2.05	0.57

Continued on next page...

Continued from previous page...

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:220:TRP:CD2	1:A:237:VAL:HB	2.40	0.56
1:A:206:TYR:HE2	1:A:211:ILE:HD13	1.70	0.56
1:B:86:ILE:CD1	1:B:155:ILE:HG12	2.35	0.56
1:B:208:ALA:HA	1:B:211:ILE:CD1	2.35	0.56
1:A:289:ASN:O	1:A:293:HIS:HB2	2.06	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:B:52:TRP:HB2	1:B:79:TYR:CE1	2.40	0.56
1:A:695:ARG:HG3	1:A:704:TYR:HE2	1.70	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:B:492:GLN:HB2	1:B:522:LYS:HE2	1.88	0.56
1:A:633:MSE:HG2	1:A:683:VAL:HG21	1.87	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:B:532:TYR:OH	1:B:615:HIS:HE1	1.89	0.55
1:A:380:GLU:HA	1:A:386:TYR:HE2	1.71	0.55
1:A:478:MSE:HE3	2:A:743:SAH:C2	2.36	0.55
1:A:383:GLN:CD	1:A:383:GLN:H	2.08	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:B:86:ILE:HD13	1:B:155:ILE:HD11	1.89	0.55
1:A:406:LYS:HD2	1:A:407:THR:H	1.72	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:B:86:ILE:HG21	1:B:155:ILE:CD1	2.37	0.54
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: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:50:ILE:O	1:A:79:TYR:HB2	2.08	0.54
1:A:396:ALA:HB1	1:A:526:ILE:HD11	1.88	0.54
1:B:382:ASP:CG	1:B:669:SER:HB2	2.28	0.54
1:B:134:ASP:OD1	1:B:173:PRO:HD2	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:GLU:HG3	1:B:429:ARG:H	1.71	0.54
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:A:305:ARG:HH11	1:A:305:ARG:HG2	1.73	0.54
1:B:649:GLN:HA	1:B:655:MSE:CB	2.38	0.54
1:A:274:ILE:HG12	1:A:274:ILE:O	2.07	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:77:PHE:CE2	1:B:318:LYS:HD3	2.43	0.54
1:B:405:ARG:H	1:B:405:ARG:HD3	1.71	0.54
1:B:648:LEU:HD21	1:B:656:LEU:HG	1.90	0.54
1:B:406:LYS:HD2	1:B:407:THR:HG22	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:384:ILE:O	1:A:388:VAL:HG23	2.08	0.53
1:A:380:GLU:HA	1:A:386:TYR:CE2	2.44	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:612:THR:O	1:B:625:ARG:NH2	2.42	0.52
1:B:478:MSE:O	1:B:517:VAL:HG23	2.08	0.52
1:A:462:MSE:HG2	1:A:467:TRP:CZ2	2.44	0.52
1:A:600:TYR:O	1:A:601:ILE:HD12	2.09	0.52
1:A:533:THR:HB	1:A:612:THR:CG2	2.39	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:B:89:VAL:HG13	1:B:93:PHE:HD2	1.75	0.52
1:A:601:ILE:HD11	1:B:259:LYS:CE	2.31	0.52
1:B:544:ILE:HB	1:B:640:MSE:HE2	1.90	0.52
1:A:702:VAL:O	1:A:732:MSE:HE3	2.10	0.52
1:A:111:ASP:HB3	1:A:158:LEU:CD2	2.40	0.52
1:B:63:LEU:HD11	1:B:70:PHE:HD1	1.74	0.51
1:B:411:TYR:HD2	1:B:493:PRO:HB3	1.74	0.51
1:A:48:ILE:CG2	1:A:326:ARG:HG2	2.40	0.51
1:B:213:HIS:HB2	3:B:775:HOH:O	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:THR:N	1:B:442:LEU:HD12	2.25	0.51
1:B:220:TRP:CD1	1:B:258:TRP:HZ3	2.27	0.51
1:A:420:ILE:HD12	2:A:743:SAH:HN2	1.75	0.51
1:B:169:ARG:HD3	3:B:748:HOH:O	2.10	0.51
1:A:527:SER:HB3	1:A:616:PRO:HD3	1.92	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:B:510:SER:N	1:B:511:PRO:CD	2.74	0.51
1:A:253:LYS:O	1:B:635:ARG:NE	2.37	0.51
1:B:648:LEU:O	1:B:655:MSE:HB2	2.11	0.51
1:A:657:SER:HB3	1:A:662:THR:O	2.10	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:57:LEU:HD12	1:B:306:ALA:CB	2.29	0.51
1:B:511:PRO:CG	1:B:532:TYR:OH	2.55	0.51
1:B:501:LEU:HD22	1:B:648:LEU:HD13	1.93	0.51
1:B:245:LEU:HD13	1:B:287:HIS:CD2	2.46	0.51
1:A:310:THR:OG1	1:A:312:LYS:HA	2.11	0.51
1:A:304:LEU:HG	1:A:305:ARG:N	2.26	0.51
1:A:695:ARG:HG3	1:A:704:TYR:CE2	2.46	0.51
1:A:391:GLU:O	1:A:394:VAL:HG22	2.11	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: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:451:LYS:HG3	1:A:452:ASN:H	1.76	0.50
1:B:387:ASP:HA	1:B:423:LYS:NZ	2.27	0.50
1:A:711:LYS:HG3	1:A:717:SER:HB2	1.92	0.50
1:B:360:LEU:C	1:B:361:GLN:HG3	2.32	0.50
1:A:406:LYS:HB3	1:A:440:GLU:OE1	2.12	0.50
1:A:367:LEU:O	1:A:451:LYS:HE2	2.12	0.50
1:B:388:VAL:HA	1:B:391:GLU:HG2	1.94	0.50
1:A:59:VAL:HG13	1:A:89:VAL:HG11	1.92	0.50
1:A:310:THR:HG23	1:A:312:LYS:HG3	1.92	0.50
1:B:541:SER:OG	1:B:544:ILE:HG12	2.12	0.50
1:A:55:THR:HG22	1:A:305:ARG:HE	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:CYS:HG	1:A:182:TRP:HZ2	1.59	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:B:418:GLY:N	1:B:419:PRO:CD	2.75	0.50
1:A:248:GLU:HA	1:A:254:LEU:HD12	1.93	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:B:55:THR:HG22	1:B:56:THR:N	2.27	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:A:272:LEU:CD2	1:A:283:ILE:HG23	2.43	0.49
1:A:127:ILE:HD12	1:A:127:ILE:N	2.27	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:O	1:A:315:THR:HG22	2.12	0.49
1:A:116:ASN:HD21	1:A:417:ARG:HH12	1.60	0.49
1:B:236:GLN:CB	1:B:264:ALA:HB2	2.42	0.49
1:A:395:GLY:HA2	1:A:398:LYS:HE2	1.95	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: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:A:492:GLN:HG2	1:A:520:PHE:O	2.13	0.48
1:A:86:ILE:HG21	1:A:155:ILE:HD13	1.95	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:698:ASP:HB2	1:B:703:TRP:CZ3	2.40	0.48
1:B:405:ARG:HB2	1:B:405:ARG:NH2	2.27	0.48
1:A:300:LEU:H	1:A:300:LEU:CD1	2.23	0.48
1:B:162:THR:HG22	1:B:163:MSE:N	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:603:LEU:HB3	1:A:633:MSE:SE	2.63	0.48
1:A:714:ASN:OD1	1:A:714:ASN:N	2.38	0.48
1:A:533:THR:HG23	1:A:535:TYR:HE2	1.78	0.48
1:A:165:ILE:HG23	1:A:165:ILE:O	2.14	0.48
1:A:283:ILE:HG22	1:A:287:HIS:HB2	1.96	0.48
1:A:310:THR:O	1:A:312:LYS:HG3	2.14	0.48
1:A:649:GLN:O	1:A:649:GLN:HG3	2.14	0.48
1:A:608:LYS:HD2	1:A:629:ILE:CG2	2.43	0.48
1:A:176:ALA:HB1	1:A:226:ASN:HB3	1.96	0.48
1:B:675:ILE:HD12	1:B:675:ILE:N	2.29	0.48
1:B:380:GLU:OE2	1:B:417:ARG:HB2	2.13	0.47
1:B:271:GLY:O	1:B:272:LEU:HD13	2.13	0.47
1:A:556:LEU:HA	1:A:556:LEU:HD12	1.65	0.47
1:B:607:THR:CG2	1:B:660:PRO:HG2	2.44	0.47
1:B:360:LEU:O	1:B:361:GLN:HG3	2.13	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:B:52:TRP:CD1	1:B:74:LEU:HD13	2.50	0.47
1:B:207:ASP:O	1:B:211:ILE:HG23	2.13	0.47
1:A:305:ARG:NH1	1:A:305:ARG:HG2	2.29	0.47
1:B:531:LYS:HZ1	1:B:614:GLU:HB3	1.79	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:317:ILE:HG13	1:A:320:GLU:CD	2.34	0.47
1:A:648:LEU:HD23	1:A:656:LEU:HD12	1.96	0.47
1:A:648:LEU:O	1:A:655:MSE:HB2	2.14	0.47
1:A:55:THR:CG2	1:A:305:ARG:HE	2.27	0.47
1:A:697:VAL:HG13	1:A:702:VAL:HG22	1.97	0.47
1:A:420:ILE:O	1:A:424:ILE:HG13	2.14	0.47
1:A:191:THR:HG22	1:A:192:VAL:N	2.30	0.47
1:A:647:ASP:C	1:A:647:ASP:OD1	2.53	0.47
1:A:533:THR:O	1:A:646:PHE:HA	2.15	0.47
1:B:383:GLN:HG2	1:B:384:ILE:N	2.29	0.47
1:A:595:VAL:O	1:A:672:PRO:HD2	2.13	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:LEU:HD11	1:B:220:TRP:HB2	1.97	0.46
1:B:67:VAL:HG21	1:B:109:LEU:HD11	1.96	0.46
1:A:515:ASP:O	1:A:518:THR:HG23	2.15	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:B:56:THR:HA	1:B:59:VAL:CG2	2.45	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:162:THR:HG23	1:B:191:THR:HB	1.97	0.46
1:A:55:THR:C	1:A:57:LEU:H	2.18	0.46
1:A:367:LEU:HD13	2:A:743:SAH:HN61	1.81	0.46
1:A:186:ARG:HD3	1:A:186:ARG:HA	1.73	0.46
1:A:690:SER:HB3	1:A:692:LYS:HZ3	1.81	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:451:LYS:O	1:B:453:PRO:HD3	2.16	0.46
1:B:44:ALA:HB3	1:B:47:ARG:HD3	1.97	0.46
1:B:86:ILE:HD11	1:B:151:GLU:CG	2.43	0.46
1:A:171:SER:C	1:A:173:PRO:HD3	2.35	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:215:ASP:H	1:B:218:THR:HB	1.81	0.46
1:B:133:CYS:HB2	1:B:175:THR:OG1	2.16	0.46
1:A:277:ARG:HG3	1:A:280:GLU:CG	2.46	0.46
1:B:317:ILE:HG22	1:B:317:ILE:O	2.16	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:A:125:GLY:O	1:A:163:MSE:HG2	2.16	0.46
1:A:398:LYS:HD3	1:A:435:PHE:CZ	2.50	0.46
1:B:659:GLU:HG3	1:B:660:PRO:HD2	1.97	0.45
1:A:698:ASP:HA	3:A:798:HOH:O	2.16	0.45
1:A:168:THR:HB	1:A:204:LYS:HZ3	1.80	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:HD12	1:B:272:LEU:HA	1.75	0.45
1:B:572:GLU:HG2	1:B:573:ASP:OD1	2.16	0.45
1:A:452:ASN:C	1:A:452:ASN:OD1	2.55	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LYS:HA	1:A:164:ALA:O	2.17	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:648:LEU:CD2	1:A:656:LEU:HD12	2.46	0.45
1:A:527:SER:HB2	1:A:616:PRO:HG3	1.98	0.45
1:B:538:PRO:HD3	1:B:631:PHE:CE1	2.52	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:727:GLY:O	1:A:731:TYR:HB2	2.17	0.45
1:A:703:TRP:HA	1:A:732:MSE:CE	2.46	0.45
1:B:80:ASN:ND2	1:B:80:ASN:H	2.14	0.45
1:B:608:LYS:HB3	1:B:609:PRO:HD2	1.99	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:B:163:MSE:SE	1:B:192:VAL:HG22	2.68	0.44
1:A:703:TRP:NE1	1:A:705:GLU:HG3	2.31	0.44
1:A:50:ILE:HD13	1:A:302:ILE:HB	1.99	0.44
1:B:692:LYS:O	1:B:706:TRP:HA	2.17	0.44
1:A:537:LYS:HA	1:A:538:PRO:HD3	1.88	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:B:509:LEU:HD11	1:B:702:VAL:HB	1.99	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:B:529:PRO:HA	1:B:650:LEU:HA	1.99	0.44
1:A:636:ASN:HA	1:A:684:GLY:HA2	2.00	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:537:LYS:HA	1:B:538:PRO:HD3	1.87	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:383:GLN:NE2	1:B:383:GLN:H	2.16	0.43
1:A:290:LEU:HD23	1:A:291:LEU:HD12	2.00	0.43
1:B:501:LEU:HD12	1:B:501:LEU:N	2.33	0.43
1:A:207:ASP:C	1:A:209:PHE:H	2.21	0.43
1:A:411:TYR:CD1	1:A:447:TYR:HB2	2.54	0.43
1:B:703:TRP:HA	1:B:732:MSE:HE2	1.99	0.43
1:A:86:ILE:CD1	1:A:151:GLU:HB3	2.48	0.43
1:B:443:LYS:HE3	1:B:470:ARG:NH2	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:590:ASP:HB2	1:A:729:SER:CB	2.48	0.43
1:A:628:SER:C	1:A:629:ILE:HD13	2.39	0.43
1:A:196:LEU:HD21	1:A:220:TRP:HB2	1.99	0.43
1:A:633:MSE:HG2	1:A:683:VAL:CG2	2.48	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:B:89:VAL:HG22	1:B:93:PHE:HE2	1.84	0.43
1:A:509:LEU:CD2	1:A:509:LEU:N	2.82	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:697:VAL:HG12	1:B:698:ASP:N	2.34	0.43
1:B:211:ILE:O	1:B:211:ILE:HG13	2.18	0.43
1:B:481:LEU:N	1:B:482:PRO:CD	2.81	0.43
1:B:251:GLU:O	1:B:255:VAL:HG23	2.19	0.43
1:A:209:PHE:O	1:A:209:PHE:CG	2.72	0.43
1:B:630:GLU:C	1:B:631:PHE:CD2	2.93	0.42
1:B:288:ILE:HG23	1:B:292:LYS:HE3	2.01	0.42
1:B:122:TYR:CD1	1:B:122:TYR:N	2.84	0.42
1:A:134:ASP:HA	3:A:776:HOH:O	2.19	0.42
1:B:112:VAL:HG11	1:B:462:MSE:HE1	2.01	0.42
1:A:616:PRO:HG2	1:A:618:PHE:CZ	2.54	0.42
1:B:569:GLU:OE1	1:B:579:LYS:HE2	2.19	0.42
1:B:485:ALA:O	1:B:490:PHE:N	2.52	0.42
1:B:294:LEU:HD23	1:B:294:LEU:HA	1.82	0.42
1:A:709:GLU:HG2	1:A:719:SER:HB2	2.01	0.42
1:A:148:LEU:HD23	1:A:178:ILE:HG21	2.01	0.42
1:A:47:ARG:HD3	1:A:48:ILE:H	1.84	0.42
1:A:154:TYR:HD1	1:A:454:ASN:OD1	2.03	0.42
1:B:91:ARG:HA	1:B:105:PRO:HG2	2.00	0.42
1:A:559:ALA:HB2	1:A:576:TRP:O	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: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:A:232:GLY:O	1:A:236:GLN:HG2	2.20	0.42
1:B:273:PHE:CD1	1:B:273:PHE:N	2.88	0.42
1:A:253:LYS:HB3	1:A:253:LYS:HE2	1.75	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:405:ARG:HH21	1:A:405:ARG:HG2	1.85	0.42
1:A:128:SER:HB3	1:A:130:TRP:NE1	2.34	0.42
1:B:249:LEU:HB3	1:B:290:LEU:CD1	2.49	0.42
1:B:724:ASN:OD1	1:B:727:GLY:HA2	2.19	0.42
1:A:47:ARG:HD2	1:A:47:ARG:N	2.33	0.42
1:A:601:ILE:CD1	1:B:259:LYS:HB2	2.50	0.42
1:A:497:VAL:HA	1:A:528:ILE:O	2.20	0.42
1:A:640:MSE:C	1:A:640:MSE:SE	3.09	0.42
1:A:454:ASN:ND2	1:A:454:ASN:H	2.18	0.42
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:216:LEU:O	1:A:219:ILE:HB	2.20	0.41
1:B:212:GLU:HG3	3:B:775:HOH:O	2.20	0.41
1:B:171:SER:C	1:B:173:PRO:HD3	2.40	0.41
1:A:111:ASP:OD1	1:A:111:ASP:N	2.54	0.41
1:B:165:ILE:O	1:B:165:ILE:HG23	2.20	0.41
1:A:385:LYS:HB3	1:A:385:LYS:HE2	1.91	0.41
1:A:300:LEU:HD12	1:A:300:LEU:N	2.29	0.41
1:A:74:LEU:HD22	1:A:79:TYR:OH	2.20	0.41
1:B:295:TRP:HZ3	1:B:302:ILE:HG13	1.85	0.41
1:B:110:PRO:O	1:B:113:GLN:HG2	2.20	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:B:514:LEU:HA	1:B:514:LEU:HD23	1.89	0.41
1:B:532:TYR:CE2	1:B:615:HIS:CE1	3.09	0.41
1:A:486:LYS:HB3	1:A:486:LYS:NZ	2.36	0.41
1:A:314:ASN:O	1:A:315:THR:CB	2.69	0.41
1:A:283:ILE:HG22	1:A:287:HIS:HB3	2.00	0.41
1:A:220:TRP:CZ3	1:A:237:VAL:HB	2.55	0.41
1:A:277:ARG:CB	1:A:280:GLU:HG2	2.38	0.41
1:B:532:TYR:CE2	1:B:615:HIS:HE1	2.39	0.41
1:B:411:TYR:HB2	1:B:496:ILE:HG22	2.02	0.41
1:B:454:ASN:N	1:B:454:ASN:HD22	2.18	0.41
1:A:481:LEU:N	1:A:482:PRO:HD2	2.36	0.41
1:A:77:PHE:CE1	1:A:315:THR:O	2.74	0.41
1:A:116:ASN:HD21	1:A:417:ARG:NH1	2.19	0.41
1:A:682:ARG:HH21	1:B:221:ALA:CB	2.31	0.41
1:A:498:SER:CB	1:A:514:LEU:HD21	2.51	0.41
1:B:380:GLU:HA	1:B:386:TYR:OH	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:ILE:HD13	1:B:444:VAL:HG13	2.02	0.41
1:B:379:PHE:HD1	1:B:379:PHE:HA	1.72	0.41
1:B:658:ILE:O	1:B:658:ILE:HD13	2.21	0.41
1:B:172:SER:N	1:B:173:PRO:HD3	2.36	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:A:200:ILE:H	1:A:200:ILE:HG13	1.54	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:493:PRO:HD3	1:A:520:PHE:CE2	2.56	0.40
1:B:640:MSE:C	1:B:640:MSE:SE	3.10	0.40
1:B:114:LEU:HG	1:B:118:LEU:HD12	2.03	0.40
1:A:406:LYS:N	1:A:406:LYS:CD	2.83	0.40
1:A:709:GLU:HG2	1:A:719:SER:CB	2.51	0.40
1:A:677:LEU:HA	1:A:723:GLN:OE1	2.21	0.40
1:A:431:TYR:CE2	1:A:442:LEU:HD23	2.56	0.40
1:A:79:TYR:HD1	1:A:79:TYR:O	2.04	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: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:B:509:LEU:CD2	1:B:732:MSE:HB3	2.50	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:A:412:LEU:HB3	1:A:448:ILE:HG12	2.03	0.40
1:A:410:ILE:HD12	1:A:444:VAL:HG11	2.04	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:B:115:ARG:CG	1:B:118:LEU:HG	2.51	0.40
1:B:536:VAL:HG11	1:B:691:LEU:HD23	2.03	0.40
1:B:263:LEU:HD12	1:B:264:ALA:N	2.36	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: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
1:B:314:ASN:O	1:B:315:THR:C	2.58	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%)	17	58
1	B	643/745 (86%)	581 (90%)	56 (9%)	6 (1%)	21	64
All	All	1301/1490 (87%)	1160 (89%)	128 (10%)	13 (1%)	19	61

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%)	9	33

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	577/645 (90%)	515 (89%)	62 (11%)	8	31
All	All	1164/1290 (90%)	1042 (90%)	122 (10%)	8	32

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	-	20,28,28	1.08	2 (10%)	19,40,40	2.95	2 (10%)
2	SAH	B	743	-	20,28,28	1.10	2 (10%)	19,40,40	2.85	2 (10%)

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	-	-	0/7/31/31	0/3/3/3
2	SAH	B	743	-	-	0/7/31/31	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-N1	2.40	1.38	1.33
2	A	743	SAH	C2-N1	2.42	1.38	1.33
2	A	743	SAH	C2-N3	3.37	1.38	1.32
2	B	743	SAH	C2-N3	3.45	1.38	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	743	SAH	N3-C2-N1	-11.54	120.06	128.89
2	B	743	SAH	N3-C2-N1	-11.25	120.28	128.89
2	A	743	SAH	C5'-SD-CG	-4.29	89.53	102.41
2	B	743	SAH	C5'-SD-CG	-3.58	91.65	102.41

There are no chirality outliers.

There are no torsion outliers.

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

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	648/745 (86%)	-0.40	8 (1%)	81 55	12, 78, 146, 239	0
1	B	637/745 (85%)	-0.22	9 (1%)	78 51	16, 88, 162, 216	13 (2%)
All	All	1285/1490 (86%)	-0.31	17 (1%)	79 53	12, 82, 154, 239	13 (1%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	313	TYR	5.0
1	B	429	ARG	3.8
1	B	308	THR	3.6
1	A	313	TYR	3.4
1	A	311	PHE	2.8
1	A	99	SER	2.7
1	B	406	LYS	2.7
1	B	316	SER	2.4
1	B	287	HIS	2.4
1	A	327	HIS	2.3
1	A	314	ASN	2.3
1	A	713	THR	2.3
1	A	490	PHE	2.2
1	A	275	SER	2.1
1	B	115	ARG	2.1
1	B	470	ARG	2.1
1	B	519	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	SAH	B	743	26/26	0.93	0.20	-0.23	85,97,121,203	0
2	SAH	A	743	26/26	0.96	0.14	-0.76	70,75,88,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.