



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 1, 2020 – 11:34 pm BST

PDB ID : 1A6E
Title : THERMOSOME-MG-ADP-ALF3 COMPLEX
Authors : Ditzel, L.; Loewe, J.; Stock, D.; Stetter, K.-O.; Huber, H.; Huber, R.; Steinbacher, S.
Deposited on : 1998-02-24
Resolution : 3.20 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

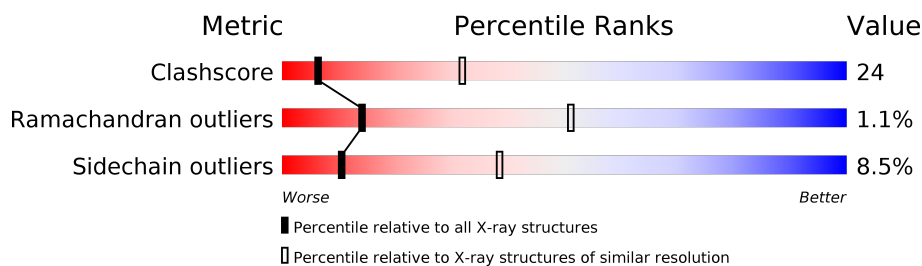
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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))
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	545	
2	B	543	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9390 atoms, of which 1742 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 THERMOSOME (ALPHA SUBUNIT).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	503	Total	C	H	N	O	S	884	0	0
			4668	2356	884	662	752	14			

- Molecule 2 is a protein called THERMOSOME (BETA SUBUNIT).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	502	Total	C	H	N	O	S	858	0	0
			4656	2370	858	651	758	19			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

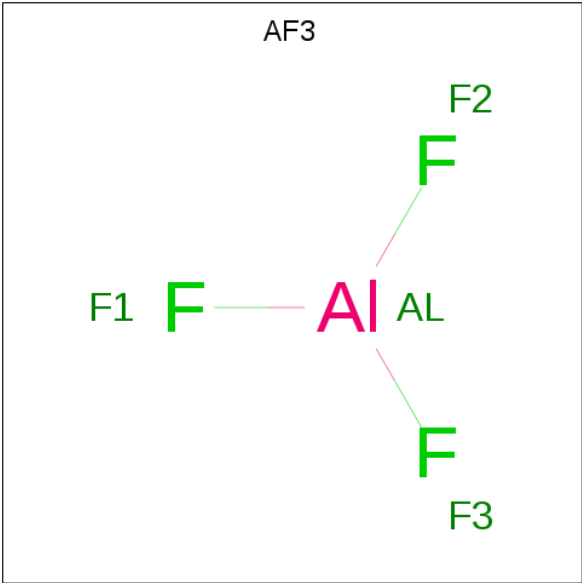
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 5 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Al	F	0	0
			4	1	3		
5	B	1	Total	Al	F	0	0
			4	1	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		
6	B	1	Total	O	0	0
			1	1		

I511	A424	E346	I272	L172
I512	A425	R347	I273	Y177
I513	K426	V348	L274	E178
I514	I427	E349	R275	E185
I515	R430	Q350	E276	E192
I516	Q431	V351	I277	
	Q432	K352	V278	
I519	L433	V353		
I520	E436	G354	I281	F195
A521	E355	E356		D196
THR	D440	Y357	V284	I197
LYS	A441	K358	I287	I198
SER	I442	T359		Q199
SER	E443	F360	I290	V200
SER	E444	V361	T291	K203
SER	E445	T362	Q292	Q204
ASN	P446	G363	K293	
PRO	A450			A207
PRO		R366	D286	L208
LYS	L455	P367	D297	D209
SER	D456	K368	M298	D210
GLY	P457	A369	A299	T211
SER	I458	V370	Q300	Q212
SER		S371	H301	L213
SER	P459	I372	Y302	I214
GLU	I460	L373	L303	N215
SER	L461	V374	S304	G216
SER	L462	R375	R305	I217
GLU		G376		I218
ASP	I472	I389	A310	V219
	K473	T390	V311	D220
	T474	D391	R312	K221
	Y475		R313	E222
	G476		V314	K223
	I477	R394	K315	V224
		V395	K316	
	I484	V396	S317	Y228
	M487	A399	L322	V232
	V488	L400		
	K489	E401	A325	A235
	I490	D402	T326	K236
	G491		G327	I237
	V492	Y405	A328	A238
		A406	S329	L239
	P495	A407	I330	L240
	I496	G408	V331	D241
	R497	G409	S332	A242
	V498		T333	P243
	G499	T412	I334	L244
				E245
	K500	E415	I337	I246
	Q501	I416	S338	K247
	A502		S339	K248
	I503	L420	S340	P249
	T507	R421	D341	E250
		S422	L342	
	A510	Y423	G343	R256

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	167.80 Å 167.80 Å 202.30 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.20	Depositor
% Data completeness (in resolution range)	92.5 (8.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.181 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9390	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, AF3

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	0.49	0/3812	0.74	2/5139 (0.0%)
2	B	0.52	0/3834	0.74	1/5166 (0.0%)
All	All	0.50	0/7646	0.74	3/10305 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	244	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	57	ASP	N-CA-C	5.18	125.00	111.00
1	A	160	SER	N-CA-C	5.15	124.91	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3784	884	3935	191	0
2	B	3798	858	3892	195	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	27	0	12	1	0
4	B	27	0	12	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
All	All	7648	1742	7851	374	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 24.

All (374) 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:218:ILE:HD11	1:A:321:LEU:HD11	1.22	1.11
2:B:172:LEU:HD22	2:B:389:ILE:HD11	1.46	0.96
1:A:281:LYS:HD2	1:A:305:GLU:HG3	1.48	0.95
2:B:50:LEU:HB2	2:B:58:VAL:HG13	1.48	0.93
2:B:64:VAL:HG22	2:B:95:THR:HG21	1.49	0.93
2:B:243:PRO:HD3	2:B:293:LYS:HD2	1.52	0.88
2:B:503:ILE:O	2:B:507:THR:HG23	1.75	0.87
1:A:69:LYS:HE2	1:A:86:LYS:HG2	1.56	0.86
2:B:152:LEU:HD11	2:B:400:LEU:HD13	1.60	0.83
2:B:421:ARG:HG3	2:B:421:ARG:HH11	1.45	0.82
2:B:489:LYS:HD3	2:B:490:ASN:HD22	1.45	0.81
1:A:163:ASN:HD21	2:B:127:ARG:HH22	1.32	0.78
2:B:425:GLN:OE1	2:B:426:LYS:HG3	1.84	0.77
2:B:48:LYS:HG3	2:B:66:ILE:HD13	1.66	0.76
1:A:51:LEU:HA	2:B:520:ILE:O	1.86	0.76
2:B:510:ALA:O	2:B:514:LEU:HB2	1.86	0.76
1:A:328:LYS:HB2	1:A:340:VAL:HB	1.68	0.75
1:A:512:ILE:HA	1:A:515:ILE:HD12	1.69	0.75
2:B:118:HIS:HD2	2:B:120:THR:H	1.35	0.75
2:B:409:GLY:O	2:B:477:ILE:HD12	1.87	0.75
1:A:17:ARG:HG3	1:A:519:ILE:HG12	1.69	0.74
2:B:185:GLU:HB2	2:B:192:TYR:CD1	2.22	0.73
1:A:478:LEU:H	1:A:478:LEU:HD23	1.53	0.73
1:A:51:LEU:HD11	1:A:67:ILE:HA	1.71	0.72
1:A:405:LEU:HD13	1:A:411:VAL:HG11	1.71	0.72
1:A:132:ASN:O	1:A:136:LYS:HD3	1.89	0.71
1:A:156:LEU:HD13	1:A:172:ALA:HB2	1.71	0.71
1:A:51:LEU:HD23	2:B:520:ILE:HG13	1.71	0.71
2:B:87:GLN:HG2	2:B:95:THR:HA	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:246:ILE:HD12	2:B:246:ILE:O	1.91	0.70
1:A:405:LEU:HD12	1:A:498:LYS:HG3	1.74	0.69
2:B:37:VAL:HG13	2:B:96:THR:HG23	1.75	0.69
1:A:154:ILE:HD13	1:A:492:VAL:HG23	1.73	0.69
2:B:458:ILE:O	2:B:462:LEU:HD22	1.94	0.68
1:A:406:TRP:O	1:A:411:VAL:HG23	1.94	0.68
1:A:75:HIS:ND1	1:A:76:PRO:HD2	2.09	0.68
1:A:486:MET:SD	1:A:491:VAL:HG21	2.34	0.67
1:A:261:LYS:HE2	1:A:261:LYS:HA	1.76	0.67
1:A:132:ASN:ND2	1:A:135:ARG:HH12	1.93	0.66
2:B:80:MET:O	2:B:83:VAL:HB	1.95	0.66
1:A:223:VAL:CG1	1:A:311:ARG:HG2	2.25	0.66
2:B:241:ASP:HB2	2:B:330:ILE:CG2	2.25	0.66
1:A:218:ILE:HD11	1:A:321:LEU:CD1	2.14	0.65
1:A:222:LYS:HD2	1:A:227:MET:HB2	1.78	0.65
2:B:83:VAL:O	2:B:86:THR:HG22	1.96	0.65
1:A:159:LEU:HD21	1:A:391:ALA:HB2	1.76	0.65
2:B:185:GLU:HB2	2:B:192:TYR:CE1	2.31	0.65
1:A:275:GLN:O	1:A:279:LYS:HG2	1.97	0.65
1:A:163:ASN:ND2	2:B:127:ARG:HH22	1.94	0.65
1:A:201:LYS:HB2	1:A:381:VAL:CG1	2.27	0.65
1:A:406:TRP:CH2	1:A:487:LYS:HD2	2.32	0.64
2:B:237:ILE:HD13	2:B:326:THR:HG21	1.79	0.64
1:A:245:ILE:HG12	1:A:273:PHE:CZ	2.31	0.64
2:B:65:THR:O	2:B:69:GLU:HB2	1.97	0.64
1:A:138:ILE:HD11	1:A:499:THR:CG2	2.27	0.64
1:A:204:GLY:HA3	1:A:374:ARG:NH1	2.12	0.64
1:A:218:ILE:CD1	1:A:321:LEU:HD11	2.14	0.63
1:A:51:LEU:CD2	2:B:520:ILE:HG13	2.28	0.63
1:A:213:ILE:HG12	1:A:359:PHE:HE2	1.63	0.63
1:A:352:ILE:HG21	1:A:372:LEU:HD21	1.81	0.62
1:A:231:VAL:HG12	1:A:234:ALA:HB2	1.81	0.62
2:B:219:VAL:HB	2:B:359:THR:HG23	1.81	0.62
2:B:64:VAL:HG22	2:B:95:THR:CG2	2.28	0.62
1:A:67:ILE:O	1:A:71:MET:HB2	1.99	0.62
2:B:460:ILE:HG23	2:B:484:ILE:HD11	1.80	0.62
2:B:217:ILE:O	2:B:361:VAL:HG12	1.98	0.61
1:A:93:GLY:HA3	1:A:393:ARG:HD2	1.82	0.61
2:B:402:ASP:OD2	2:B:497:ARG:HB2	2.00	0.61
1:A:131:VAL:HB	1:A:506:VAL:HG21	1.83	0.61
1:A:417:MET:SD	1:A:468:GLU:HA	2.41	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:445:ILE:HB	2:B:446:PRO:HD3	1.82	0.60
1:A:278:GLU:O	1:A:282:LYS:HG3	2.02	0.60
2:B:30:ALA:HB1	2:B:80:MET:HE1	1.83	0.60
1:A:50:MET:HE2	1:A:60:ILE:HD11	1.83	0.60
2:B:130:SER:HB2	2:B:507:THR:HG21	1.84	0.59
1:A:112:THR:HG22	1:A:116:GLN:HE21	1.66	0.59
2:B:512:MET:O	2:B:516:ILE:HG13	2.02	0.59
2:B:214:ILE:HG13	2:B:218:ILE:HD11	1.84	0.59
2:B:352:LYS:HG3	2:B:356:ASP:O	2.03	0.59
1:A:17:ARG:HB2	1:A:519:ILE:HG23	1.85	0.59
1:A:291:GLN:OE1	1:A:315:LYS:HD3	2.03	0.59
2:B:137:ILE:HG22	2:B:496:ILE:HG13	1.84	0.58
2:B:144:ILE:HG12	2:B:405:TYR:HD2	1.67	0.58
1:A:205:GLY:O	1:A:206:SER:HB2	2.02	0.58
1:A:406:TRP:CZ3	1:A:487:LYS:HA	2.38	0.58
1:A:137:ILE:O	1:A:141:ILE:HG12	2.03	0.58
1:A:152:ARG:O	1:A:156:LEU:HD22	2.03	0.58
2:B:424:ALA:HB1	2:B:432:GLN:HG3	1.86	0.58
2:B:487:MET:HE3	2:B:492:VAL:HG21	1.86	0.58
2:B:499:GLY:O	2:B:503:ILE:HG23	2.04	0.57
1:A:218:ILE:HG22	1:A:220:LYS:HB2	1.86	0.57
1:A:445:PRO:HB2	1:A:460:LEU:HD21	1.86	0.57
2:B:212:GLN:HG3	2:B:214:ILE:HD11	1.85	0.57
2:B:67:LEU:HD21	2:B:99:VAL:HG21	1.85	0.57
2:B:68:LYS:HG2	2:B:85:LYS:HE2	1.86	0.57
2:B:133:ALA:HB3	2:B:503:ILE:HD13	1.86	0.57
2:B:107:GLN:O	2:B:110:GLN:HB3	2.05	0.57
2:B:199:GLN:HB3	2:B:371:SER:OG	2.03	0.57
1:A:201:LYS:HB2	1:A:381:VAL:HG11	1.86	0.57
1:A:412:GLU:OE2	1:A:498:LYS:HE3	2.05	0.57
1:A:48:ASP:OD1	1:A:62:ASN:HB2	2.03	0.57
2:B:301:HIS:CE1	2:B:305:ARG:HD2	2.39	0.57
2:B:239:LEU:HD22	2:B:328:ALA:HB3	1.86	0.57
1:A:65:ALA:HB1	1:A:69:LYS:HE3	1.87	0.56
2:B:132:GLU:OE2	2:B:135:ARG:HD3	2.05	0.56
2:B:152:LEU:CD1	2:B:400:LEU:HD13	2.33	0.56
1:A:289:LEU:HD23	1:A:321:LEU:HD13	1.88	0.56
1:A:61:SER:HB2	1:A:386:ARG:NH1	2.20	0.56
2:B:347:ARG:CB	2:B:347:ARG:HH11	2.18	0.56
2:B:421:ARG:HG3	2:B:421:ARG:NH1	2.18	0.56
1:A:405:LEU:CD1	1:A:498:LYS:HG3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:472:ASN:HB3	2:B:475:TYR:CD1	2.40	0.56
1:A:204:GLY:HA3	1:A:374:ARG:CZ	2.36	0.55
1:A:450:GLU:HG2	1:A:456:PRO:HG3	1.88	0.55
1:A:206:SER:HB3	1:A:209:ASP:HB2	1.88	0.55
2:B:222:GLU:HB2	2:B:350:GLN:OE1	2.06	0.55
2:B:399:ALA:HB2	2:B:495:PRO:HG3	1.88	0.55
2:B:27:ILE:O	2:B:31:ILE:HG13	2.06	0.55
1:A:58:ILE:HD13	2:B:79:MET:SD	2.47	0.55
2:B:140:ILE:HG21	2:B:415:GLU:HG2	1.88	0.55
1:A:235:LYS:HE2	1:A:341:LEU:HD12	1.89	0.55
2:B:87:GLN:HE22	2:B:502:ALA:N	2.05	0.55
1:A:486:MET:HB3	1:A:491:VAL:HG22	1.89	0.54
1:A:510:THR:O	1:A:514:ARG:HG3	2.08	0.54
2:B:118:HIS:CD2	2:B:120:THR:H	2.20	0.54
2:B:64:VAL:HA	2:B:84:SER:OG	2.06	0.54
1:A:196:ASN:HD21	1:A:323:LYS:HE2	1.72	0.54
1:A:192:VAL:HG21	1:A:396:ALA:HB1	1.89	0.54
1:A:286:ASN:C	1:A:307:ILE:HG23	2.28	0.54
2:B:292:GLN:HE22	2:B:316:LYS:HD3	1.73	0.54
2:B:236:LYS:H	2:B:287:ASN:HB2	1.72	0.54
2:B:292:GLN:O	2:B:313:ARG:HA	2.08	0.54
2:B:241:ASP:HB2	2:B:330:ILE:HG22	1.89	0.54
2:B:511:ILE:O	2:B:515:ARG:HG3	2.07	0.53
1:A:201:LYS:HD2	1:A:381:VAL:HG12	1.89	0.53
2:B:292:GLN:NE2	2:B:316:LYS:HD3	2.23	0.53
1:A:281:LYS:CD	1:A:305:GLU:HG3	2.31	0.53
2:B:200:VAL:HG13	2:B:372:ILE:HB	1.90	0.53
1:A:17:ARG:HH21	1:A:19:GLN:HG3	1.73	0.53
2:B:232:VAL:HG22	2:B:348:VAL:HB	1.91	0.53
1:A:223:VAL:HG12	1:A:311:ARG:HG2	1.90	0.52
1:A:144:LYS:O	1:A:145:SER:HB2	2.08	0.52
1:A:200:ASP:O	1:A:373:ILE:HG13	2.09	0.52
1:A:427:GLY:O	1:A:431:GLN:HB2	2.09	0.52
1:A:486:MET:SD	1:A:491:VAL:CG2	2.96	0.52
2:B:165:ALA:HB1	2:B:172:LEU:CD1	2.40	0.52
1:A:486:MET:HB3	1:A:491:VAL:CG2	2.40	0.52
1:A:233:ASN:N	1:A:345:GLU:O	2.39	0.52
1:A:127:TYR:O	1:A:131:VAL:HG12	2.10	0.52
2:B:366:ASN:ND2	2:B:368:LYS:H	2.07	0.52
1:A:138:ILE:HD11	1:A:499:THR:HG22	1.91	0.52
2:B:347:ARG:CG	2:B:347:ARG:HH11	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:432:GLN:O	2:B:436:GLU:HG3	2.09	0.52
2:B:446:PRO:HB2	2:B:461:LEU:HD21	1.91	0.52
1:A:217:VAL:HG22	1:A:357:MET:HE2	1.93	0.51
2:B:241:ASP:HB3	2:B:332:SER:OG	2.10	0.51
1:A:192:VAL:CG2	1:A:396:ALA:HB1	2.41	0.51
1:A:426:VAL:HG12	1:A:427:GLY:N	2.26	0.51
2:B:245:GLU:HA	2:B:274:LEU:HD21	1.92	0.51
2:B:334:ILE:HD12	2:B:334:ILE:H	1.75	0.51
1:A:174:LEU:HD22	1:A:212:PHE:HB2	1.92	0.51
1:A:192:VAL:HG23	1:A:192:VAL:O	2.11	0.51
1:A:291:GLN:HB2	1:A:318:MET:HG3	1.92	0.51
2:B:239:LEU:HD22	2:B:328:ALA:CB	2.41	0.51
2:B:338:SER:O	2:B:341:ASP:HB2	2.11	0.51
2:B:346:GLU:HB2	2:B:363:GLY:HA3	1.93	0.51
1:A:31:ALA:O	1:A:34:ILE:HG22	2.12	0.50
1:A:166:LEU:HD22	1:A:166:LEU:N	2.26	0.50
1:A:177:LYS:HD3	1:A:212:PHE:CD2	2.46	0.50
2:B:237:ILE:HG22	2:B:239:LEU:HD13	1.91	0.50
1:A:44:PRO:O	1:A:161:GLY:HA2	2.10	0.50
1:A:213:ILE:HG12	1:A:359:PHE:CE2	2.46	0.50
1:A:406:TRP:O	1:A:410:ALA:HB3	2.10	0.50
1:A:255:GLN:NE2	2:B:256:ARG:HB2	2.26	0.50
2:B:490:ASN:N	2:B:490:ASN:HD22	2.08	0.50
2:B:47:ASP:OD1	2:B:61:ASN:HB2	2.12	0.50
1:A:138:ILE:CG2	1:A:415:LEU:HD11	2.42	0.50
2:B:62:ASP:O	2:B:66:ILE:HG13	2.11	0.50
1:A:377:THR:O	1:A:378:ASP:HB2	2.12	0.50
1:A:224:HIS:CE1	1:A:226:LYS:HB2	2.47	0.50
1:A:25:ARG:O	1:A:29:GLU:HG2	2.12	0.50
2:B:328:ALA:HB2	2:B:343:GLY:HA3	1.93	0.50
1:A:422:TYR:O	1:A:426:VAL:HG23	2.11	0.50
2:B:50:LEU:HB2	2:B:58:VAL:CG1	2.32	0.50
2:B:331:VAL:HG21	2:B:337:ILE:HG13	1.93	0.50
1:A:444:ILE:HB	1:A:445:PRO:HD3	1.94	0.49
2:B:134:LYS:HG3	2:B:503:ILE:HD11	1.94	0.49
2:B:456:ASP:O	2:B:460:ILE:HG12	2.12	0.49
2:B:423:TYR:HA	2:B:426:LYS:HD2	1.95	0.49
1:A:146:THR:HG22	1:A:402:GLY:HA2	1.94	0.49
1:A:253:LYS:NZ	1:A:253:LYS:HB2	2.27	0.49
1:A:198:LYS:O	1:A:370:SER:HA	2.11	0.49
1:A:371:ILE:HD12	1:A:392:ILE:HD11	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:ALA:HB1	2:B:80:MET:CE	2.43	0.49
1:A:397:ILE:HG12	1:A:496:ARG:NH2	2.28	0.49
2:B:195:PHE:C	2:B:197:ASN:H	2.16	0.49
1:A:206:SER:C	1:A:208:ASN:H	2.16	0.49
2:B:58:VAL:HG11	2:B:69:GLU:HG2	1.93	0.49
1:A:305:GLU:HA	1:A:305:GLU:OE1	2.12	0.49
1:A:73:VAL:HG21	1:A:82:VAL:HG21	1.95	0.48
2:B:237:ILE:CG2	2:B:239:LEU:HD13	2.43	0.48
1:A:41:THR:HB	1:A:62:ASN:ND2	2.28	0.48
2:B:274:LEU:HD22	2:B:299:ALA:HB2	1.95	0.48
2:B:423:TYR:CZ	2:B:427:ILE:HG13	2.48	0.48
2:B:441:ALA:O	2:B:444:GLU:HG2	2.13	0.48
2:B:64:VAL:CG2	2:B:95:THR:HG21	2.32	0.48
1:A:261:LYS:HE2	1:A:261:LYS:CA	2.41	0.48
1:A:51:LEU:HD13	1:A:70:GLU:HB2	1.95	0.48
2:B:67:LEU:HB3	2:B:81:VAL:HG13	1.96	0.48
1:A:128:ARG:HG3	1:A:132:ASN:OD1	2.14	0.48
1:A:51:LEU:CD1	1:A:70:GLU:HB2	2.44	0.48
2:B:165:ALA:HB1	2:B:172:LEU:HD12	1.96	0.48
2:B:296:ASP:O	2:B:300:GLN:HG3	2.14	0.48
2:B:325:ALA:O	2:B:366:ASN:HB3	2.14	0.48
1:A:138:ILE:HD11	1:A:499:THR:HG23	1.95	0.47
1:A:210:THR:HG23	1:A:373:ILE:HA	1.96	0.47
1:A:443:ILE:O	1:A:443:ILE:HD13	2.15	0.47
2:B:34:SER:HA	2:B:99:VAL:HG12	1.97	0.47
1:A:405:LEU:HB3	1:A:411:VAL:CG2	2.44	0.47
2:B:64:VAL:HG21	2:B:88:ASP:OD1	2.13	0.47
1:A:278:GLU:HG2	1:A:282:LYS:HD2	1.97	0.47
1:A:463:LEU:HD11	1:A:474:VAL:O	2.15	0.47
1:A:477:ASP:HB3	1:A:480:ASN:HB2	1.96	0.47
2:B:137:ILE:HG12	2:B:416:ILE:HD11	1.95	0.47
2:B:337:ILE:HG23	2:B:337:ILE:O	2.14	0.47
1:A:405:LEU:HD13	1:A:411:VAL:CG1	2.44	0.47
1:A:477:ASP:HB2	1:A:484:GLY:HA3	1.97	0.47
2:B:513:ILE:HA	2:B:516:ILE:HD12	1.97	0.47
1:A:131:VAL:CB	1:A:506:VAL:HG21	2.45	0.47
1:A:351:LYS:HE3	1:A:353:GLY:O	2.15	0.47
2:B:152:LEU:HD11	2:B:400:LEU:CD1	2.38	0.47
2:B:407:ALA:O	2:B:412:THR:HG22	2.14	0.47
2:B:158:THR:HG23	4:B:998:ADP:C8	2.50	0.47
2:B:136:VAL:O	2:B:140:ILE:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:ARG:HB3	1:A:474:VAL:HG23	1.97	0.46
2:B:185:GLU:HB2	2:B:192:TYR:HD1	1.75	0.46
1:A:130:ALA:HB2	1:A:434:ILE:HG23	1.96	0.46
1:A:78:ALA:O	1:A:82:VAL:HG23	2.15	0.46
2:B:221:LYS:HG3	2:B:314:VAL:HG22	1.97	0.46
2:B:492:VAL:O	2:B:492:VAL:HG23	2.14	0.46
1:A:405:LEU:HB3	1:A:411:VAL:HG22	1.97	0.46
1:A:256:ILE:HG23	1:A:261:LYS:HB2	1.97	0.46
2:B:199:GLN:O	2:B:371:SER:HA	2.14	0.46
2:B:51:VAL:HG13	2:B:57:ILE:HG12	1.95	0.46
1:A:154:ILE:HD13	1:A:492:VAL:CG2	2.44	0.46
1:A:69:LYS:HG2	1:A:86:LYS:HD3	1.97	0.46
2:B:132:GLU:O	2:B:136:VAL:HG23	2.16	0.46
2:B:315:LYS:HD2	2:B:317:SER:OG	2.15	0.46
2:B:149:LYS:HD2	2:B:177:TYR:CE2	2.50	0.46
1:A:308:TYR:OH	1:A:349:GLU:HB2	2.16	0.46
1:A:94:ASP:OD1	4:A:898:ADP:O2B	2.34	0.46
1:A:235:LYS:HB3	1:A:341:LEU:HD13	1.98	0.46
1:A:224:HIS:HE1	1:A:226:LYS:HB2	1.80	0.45
1:A:145:SER:HB3	1:A:404:PHE:HE2	1.81	0.45
2:B:67:LEU:HD23	2:B:84:SER:OG	2.16	0.45
2:B:207:ALA:O	2:B:210:ASP:HB2	2.16	0.45
2:B:278:VAL:HG21	2:B:302:TYR:HB2	1.99	0.45
1:A:222:LYS:HE2	1:A:227:MET:O	2.17	0.45
1:A:294:ILE:HG13	1:A:311:ARG:HB3	1.99	0.45
1:A:491:VAL:O	1:A:491:VAL:HG23	2.16	0.45
1:A:409:GLY:CA	1:A:445:PRO:HG3	2.46	0.45
1:A:50:MET:O	2:B:519:VAL:HA	2.16	0.45
2:B:370:VAL:HG22	2:B:371:SER:N	2.32	0.45
1:A:222:LYS:CD	1:A:227:MET:HB2	2.46	0.45
2:B:118:HIS:CD2	2:B:120:THR:OG1	2.70	0.45
2:B:217:ILE:O	2:B:361:VAL:CG1	2.65	0.45
1:A:20:GLY:N	1:A:516:ASP:O	2.50	0.45
1:A:84:VAL:HG12	1:A:508:VAL:HG21	1.99	0.45
2:B:408:GLY:O	2:B:487:MET:HG3	2.17	0.44
1:A:269:GLU:O	1:A:272:THR:HB	2.17	0.44
1:A:186:ARG:O	1:A:188:GLY:N	2.51	0.44
1:A:446:ARG:HB2	1:A:460:LEU:HD11	1.99	0.44
2:B:219:VAL:HB	2:B:359:THR:CG2	2.46	0.44
1:A:18:GLU:O	1:A:517:ASP:HA	2.17	0.44
1:A:266:LEU:HD12	2:B:249:PRO:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:290:ILE:HG12	2:B:311:VAL:HG22	1.99	0.44
1:A:382:SER:O	1:A:385:GLU:HB3	2.17	0.44
2:B:489:LYS:HD3	2:B:490:ASN:ND2	2.22	0.44
2:B:472:ASN:O	2:B:474:THR:N	2.51	0.44
2:B:93:ASP:O	2:B:498:VAL:HG13	2.17	0.44
2:B:68:LYS:HE3	2:B:85:LYS:HG2	2.00	0.44
1:A:460:LEU:HA	1:A:460:LEU:HD23	1.82	0.43
2:B:23:MET:SD	2:B:113:ILE:HD13	2.58	0.43
2:B:224:VAL:HG12	2:B:228:MET:SD	2.58	0.43
2:B:211:THR:HG23	2:B:374:VAL:HA	2.00	0.43
1:A:201:LYS:HA	1:A:373:ILE:O	2.18	0.43
1:A:406:TRP:CZ2	1:A:487:LYS:HD2	2.53	0.43
1:A:167:SER:O	1:A:170:PHE:N	2.51	0.43
2:B:477:ILE:O	4:B:998:ADP:H2	2.01	0.43
1:A:56:GLY:O	1:A:57:ASP:HB2	2.17	0.43
2:B:152:LEU:HA	2:B:152:LEU:HD23	1.82	0.43
2:B:352:LYS:HD3	2:B:357:TYR:CZ	2.54	0.43
1:A:223:VAL:HG23	1:A:227:MET:HE1	2.00	0.43
1:A:57:ASP:HB3	1:A:58:ILE:H	1.59	0.43
2:B:137:ILE:HG22	2:B:496:ILE:CG1	2.49	0.43
2:B:77:ALA:O	2:B:81:VAL:HG23	2.19	0.43
1:A:98:THR:O	1:A:102:LEU:HB2	2.19	0.43
1:A:186:ARG:HG3	1:A:191:ILE:HD11	2.00	0.43
2:B:212:GLN:HG3	2:B:214:ILE:CD1	2.49	0.43
2:B:284:VAL:HG22	2:B:339:SER:CA	2.49	0.43
1:A:58:ILE:HD11	2:B:75:PRO:HA	2.00	0.43
2:B:240:LEU:HA	2:B:331:VAL:O	2.19	0.43
1:A:266:LEU:CD1	2:B:249:PRO:HG3	2.49	0.42
1:A:474:VAL:HA	1:A:484:GLY:O	2.19	0.42
2:B:244:LEU:O	2:B:245:GLU:HG3	2.19	0.42
1:A:183:ALA:HB2	1:A:192:VAL:HG12	1.99	0.42
1:A:288:VAL:HG23	1:A:307:ILE:HG21	2.01	0.42
1:A:455:ASP:HA	1:A:456:PRO:HD3	1.80	0.42
1:A:17:ARG:HG3	1:A:17:ARG:HH11	1.84	0.42
1:A:477:ASP:N	1:A:482:GLY:O	2.52	0.42
1:A:17:ARG:CG	1:A:519:ILE:HG12	2.45	0.42
1:A:186:ARG:HG3	1:A:191:ILE:CD1	2.49	0.42
2:B:130:SER:CB	2:B:507:THR:HG21	2.48	0.42
2:B:232:VAL:HG23	2:B:235:ALA:HB2	2.02	0.42
2:B:430:ARG:HA	2:B:433:LEU:HD13	2.01	0.42
1:A:138:ILE:HA	1:A:141:ILE:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:VAL:HG21	1:A:301:TYR:HB2	2.00	0.42
2:B:106:LEU:HD12	2:B:106:LEU:HA	1.86	0.42
2:B:133:ALA:O	2:B:137:ILE:HG13	2.20	0.42
2:B:297:ASP:O	2:B:300:GLN:HB2	2.19	0.42
2:B:457:PRO:O	2:B:461:LEU:HB2	2.20	0.42
1:A:58:ILE:HG21	2:B:79:MET:SD	2.59	0.42
2:B:484:ILE:HD12	2:B:484:ILE:N	2.35	0.42
2:B:487:MET:SD	2:B:492:VAL:HG22	2.60	0.42
2:B:50:LEU:HD13	2:B:69:GLU:HG2	2.02	0.42
1:A:327:ALA:HB2	1:A:342:GLY:N	2.35	0.41
1:A:376:GLY:O	1:A:378:ASP:N	2.53	0.41
1:A:197:ILE:HG21	1:A:392:ILE:HD13	2.02	0.41
2:B:91:VAL:HG21	2:B:498:VAL:HA	2.01	0.41
2:B:221:LYS:O	2:B:359:THR:HG22	2.19	0.41
1:A:243:LEU:HD11	1:A:280:ILE:HD11	2.02	0.41
1:A:397:ILE:HD13	1:A:397:ILE:HG21	1.80	0.41
1:A:69:LYS:CE	1:A:86:LYS:HG2	2.40	0.41
1:A:167:SER:O	1:A:170:PHE:HB3	2.21	0.41
1:A:242:ALA:HB2	1:A:292:LYS:HB3	2.02	0.41
1:A:230:VAL:HG23	1:A:348:GLU:HB3	2.02	0.41
1:A:324:ALA:O	1:A:363:CYS:HB3	2.20	0.41
2:B:215:ASN:O	2:B:362:THR:HG23	2.20	0.41
2:B:48:LYS:CG	2:B:66:ILE:HD13	2.46	0.41
2:B:88:ASP:HB2	2:B:95:THR:HG21	2.02	0.41
2:B:97:THR:HG22	2:B:502:ALA:HB1	2.02	0.41
2:B:144:ILE:HG12	2:B:405:TYR:CD2	2.51	0.41
2:B:298:MET:HG3	2:B:302:TYR:CE2	2.56	0.41
2:B:352:LYS:HD2	2:B:355:GLU:O	2.19	0.41
2:B:391:ASP:O	2:B:395:VAL:HG23	2.19	0.41
2:B:440:ASP:O	2:B:443:GLU:HB2	2.21	0.41
2:B:450:ALA:HA	2:B:455:LEU:HD12	2.03	0.41
2:B:236:LYS:H	2:B:287:ASN:CB	2.33	0.41
2:B:94:GLY:HA2	4:B:998:ADP:O3B	2.20	0.41
1:A:177:LYS:HD3	1:A:212:PHE:CE2	2.55	0.41
2:B:147:ASP:O	2:B:148:GLU:C	2.59	0.41
2:B:204:GLN:HA	2:B:376:GLY:O	2.21	0.41
2:B:118:HIS:HD2	2:B:120:THR:N	2.11	0.41
2:B:303:LEU:HD13	2:B:310:ALA:CB	2.51	0.41
2:B:290:ILE:HD13	2:B:322:LEU:CD1	2.50	0.41
2:B:334:ILE:N	2:B:334:ILE:HD12	2.34	0.41
2:B:284:VAL:CG2	2:B:339:SER:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:VAL:CG2	1:A:357:MET:HE2	2.49	0.41
2:B:272:ASN:O	2:B:276:GLU:HG3	2.20	0.41
1:A:119:HIS:HA	1:A:120:PRO:HD3	2.00	0.40
1:A:133:GLU:OE1	1:A:133:GLU:HA	2.20	0.40
1:A:478:LEU:H	1:A:478:LEU:CD2	2.28	0.40
2:B:24:LYS:NZ	2:B:24:LYS:HB3	2.36	0.40
2:B:390:THR:HG22	2:B:394:HIS:HD2	1.86	0.40
1:A:107:LEU:HA	1:A:107:LEU:HD23	1.85	0.40
1:A:189:LYS:O	1:A:189:LYS:HD2	2.21	0.40
2:B:195:PHE:HA	2:B:198:ILE:HD12	2.04	0.40
2:B:203:LYS:HG2	2:B:353:VAL:HG12	2.04	0.40
2:B:281:ILE:O	2:B:284:VAL:HG12	2.22	0.40
1:A:42:LEU:HD23	1:A:447:THR:CG2	2.52	0.40
1:A:53:ASP:OD1	1:A:57:ASP:HA	2.21	0.40
2:B:236:LYS:HB3	2:B:342:LEU:HD23	2.03	0.40
2:B:215:ASN:HA	2:B:370:VAL:HG23	2.04	0.40
2:B:420:LEU:HA	2:B:420:LEU:HD23	1.86	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	501/545 (92%)	450 (90%)	41 (8%)	10 (2%)	7	38
2	B	500/543 (92%)	463 (93%)	36 (7%)	1 (0%)	47	79
All	All	1001/1088 (92%)	913 (91%)	77 (8%)	11 (1%)	14	51

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	57	ASP

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Mol	Chain	Res	Type
1	A	145	SER
1	A	377	THR
1	A	378	ASP
1	A	160	SER
1	A	206	SER
1	A	207	VAL
2	B	473	LYS
1	A	203	ASN
1	A	427	GLY
1	A	375	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	411/442 (93%)	375 (91%)	36 (9%)	10	36
2	B	410/446 (92%)	376 (92%)	34 (8%)	11	40
All	All	821/888 (92%)	751 (92%)	70 (8%)	10	38

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	40	THR
1	A	52	VAL
1	A	57	ASP
1	A	59	ILE
1	A	92	VAL
1	A	102	LEU
1	A	122	VAL
1	A	135	ARG
1	A	143	GLU
1	A	156	LEU
1	A	162	LYS
1	A	166	LEU

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Mol	Chain	Res	Type
1	A	189	LYS
1	A	223	VAL
1	A	230	VAL
1	A	240	ASP
1	A	251	GLU
1	A	253	LYS
1	A	296	ASP
1	A	305	GLU
1	A	311	ARG
1	A	333	LEU
1	A	354	ASP
1	A	361	MET
1	A	380	VAL
1	A	388	LEU
1	A	393	ARG
1	A	443	ILE
1	A	464	LYS
1	A	466	ASP
1	A	467	ASP
1	A	478	LEU
1	A	496	ARG
1	A	513	LEU
1	A	516	ASP
2	B	24	LYS
2	B	54	LEU
2	B	58	VAL
2	B	67	LEU
2	B	79	MET
2	B	87	GLN
2	B	106	LEU
2	B	131	GLU
2	B	153	LEU
2	B	161	ASN
2	B	163	LYS
2	B	178	GLU
2	B	192	TYR
2	B	209	ASP
2	B	239	LEU
2	B	248	LYS
2	B	250	GLU
2	B	305	ARG
2	B	339	SER

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Mol	Chain	Res	Type
2	B	340	SER
2	B	347	ARG
2	B	366	ASN
2	B	391	ASP
2	B	396	VAL
2	B	412	THR
2	B	425	GLN
2	B	430	ARG
2	B	461	LEU
2	B	462	LEU
2	B	489	LYS
2	B	501	GLN
2	B	503	ILE
2	B	507	THR
2	B	514	LEU

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

Mol	Chain	Res	Type
1	A	22	ASN
1	A	27	ASN
1	A	109	GLN
1	A	116	GLN
1	A	163	ASN
1	A	180	ASN
1	A	196	ASN
1	A	208	ASN
1	A	233	ASN
1	A	255	GLN
1	A	267	ASN
1	A	424	ASN
1	A	431	GLN
1	A	451	ASN
1	A	480	ASN
2	B	26	ASN
2	B	35	ASN
2	B	87	GLN
2	B	108	GLN
2	B	118	HIS
2	B	292	GLN
2	B	300	GLN
2	B	301	HIS

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Mol	Chain	Res	Type
2	B	366	ASN
2	B	394	HIS
2	B	490	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z > 2$
5	AF3	B	999	3,4,6	0,3,3	0.00	-	-		
4	ADP	B	998	3,5	24,29,29	1.18	4 (16%)	29,45,45	1.44	3 (10%)
4	ADP	A	898	3,5	24,29,29	1.29	4 (16%)	29,45,45	1.39	2 (6%)
5	AF3	A	899	3,4,6	0,3,3	0.00	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	A	898	3,5	-	4/12/32/32	0/3/3/3
4	ADP	B	998	3,5	-	1/12/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	898	ADP	C2'-C1'	-3.02	1.49	1.53
4	A	898	ADP	PB-O2B	2.71	1.65	1.54
4	B	998	ADP	PB-O2B	2.58	1.64	1.54
4	B	998	ADP	O4'-C1'	2.50	1.44	1.41
4	A	898	ADP	C5-N7	-2.36	1.31	1.39
4	A	898	ADP	O4'-C1'	2.29	1.44	1.41
4	B	998	ADP	C2'-C1'	-2.21	1.50	1.53
4	B	998	ADP	C5-N7	-2.17	1.31	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	998	ADP	N3-C2-N1	-5.93	119.41	128.68
4	A	898	ADP	N3-C2-N1	-5.69	119.79	128.68
4	A	898	ADP	C4-C5-N7	-2.62	106.67	109.40
4	B	998	ADP	C4-C5-N7	-2.48	106.82	109.40
4	B	998	ADP	O3B-PB-O3A	2.03	111.45	104.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

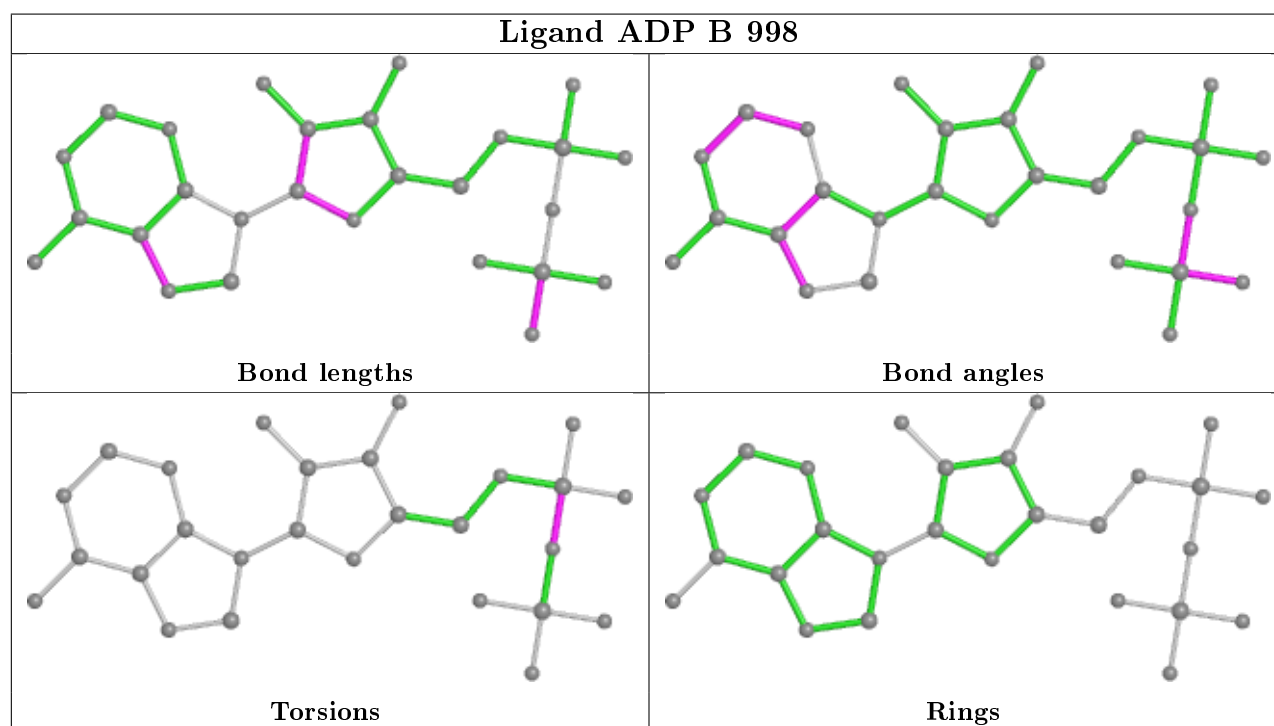
Mol	Chain	Res	Type	Atoms
4	A	898	ADP	PA-O3A-PB-O2B
4	A	898	ADP	C3'-C4'-C5'-O5'
4	A	898	ADP	PA-O3A-PB-O1B
4	A	898	ADP	PA-O3A-PB-O3B
4	B	998	ADP	PB-O3A-PA-O1A

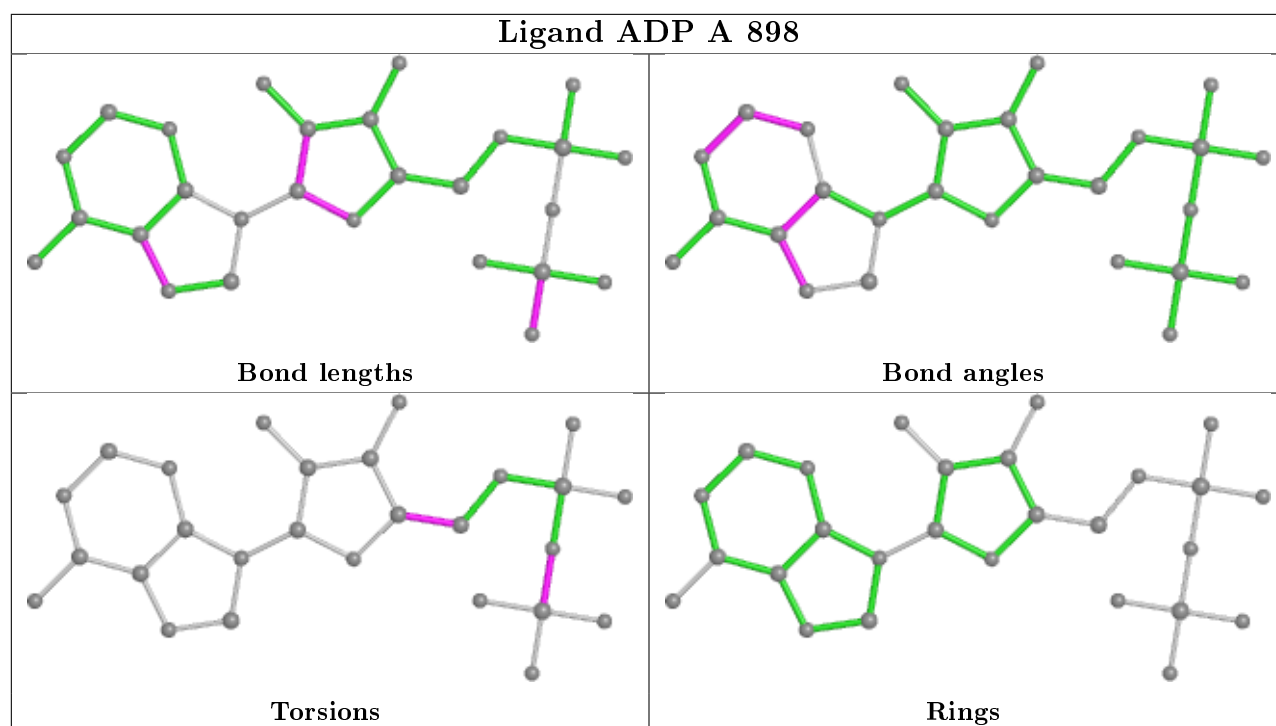
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	998	ADP	3	0
4	A	898	ADP	1	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.