



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 18, 2017 – 01:58 PM EDT

PDB ID : 3C7N
Title : Structure of the Hsp110:Hsc70 Nucleotide Exchange Complex
Authors : Schuermann, J.P.; Jiang, J.; Hart, P.J.; Sousa, R.
Deposited on : unknown
Resolution : 3.12 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

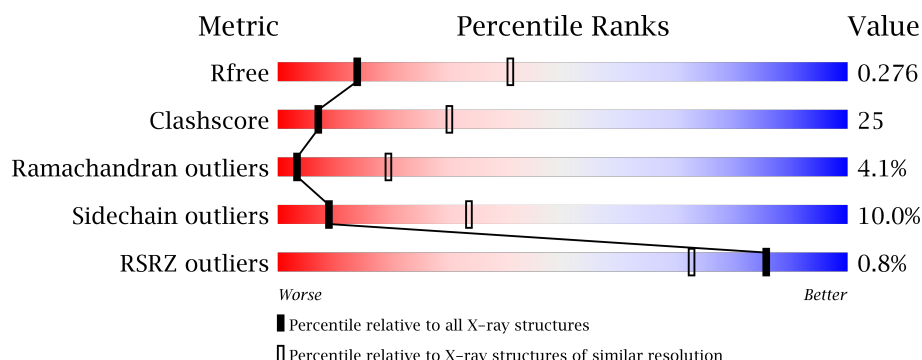
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.12 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}	100719	1000 (3.14-3.10)
Clashscore	112137	1099 (3.14-3.10)
Ramachandran outliers	110173	1060 (3.14-3.10)
Sidechain outliers	110143	1060 (3.14-3.10)
RSRZ outliers	101464	1005 (3.14-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	668	<div> <div></div> <div> <div></div> <div>54%</div> <div>37%</div> <div>6%</div> <div>.</div> </div> </div>
2	B	554	<div> <div></div> <div> <div></div> <div>49%</div> <div>40%</div> <div>9%</div> <div>..</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	A	667	-	-	-	X
4	SO4	A	668	-	-	-	X
4	SO4	A	669	-	-	-	X
4	SO4	A	670	-	-	-	X
5	BEF	A	671	-	-	-	X
7	CL	B	555	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9368 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 Heat shock protein homolog SSE1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	649	Total	C	N	O	S	0	0	0
			5103	3227	853	1010	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP P32589
A	0	PRO	-	EXPRESSION TAG	UNP P32589

- Molecule 2 is a protein called Heat shock cognate.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	540	Total	C	N	O	S	0	0	0
			4182	2621	726	824	11			

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

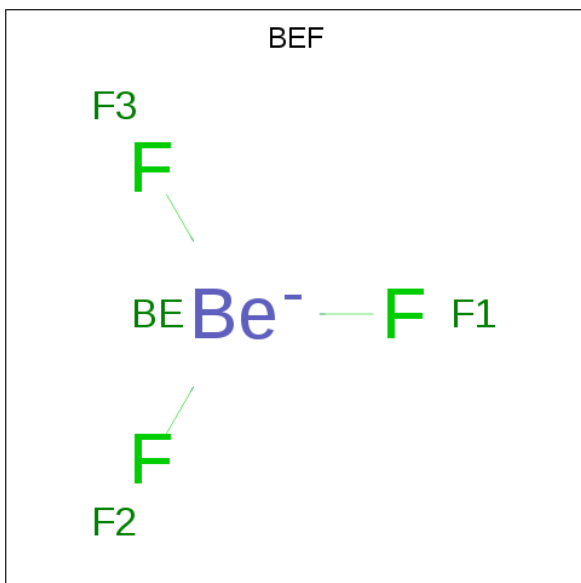
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



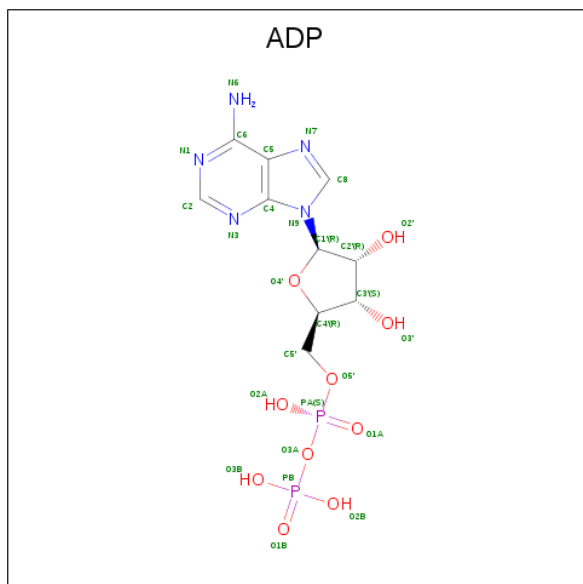
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF₃).



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

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

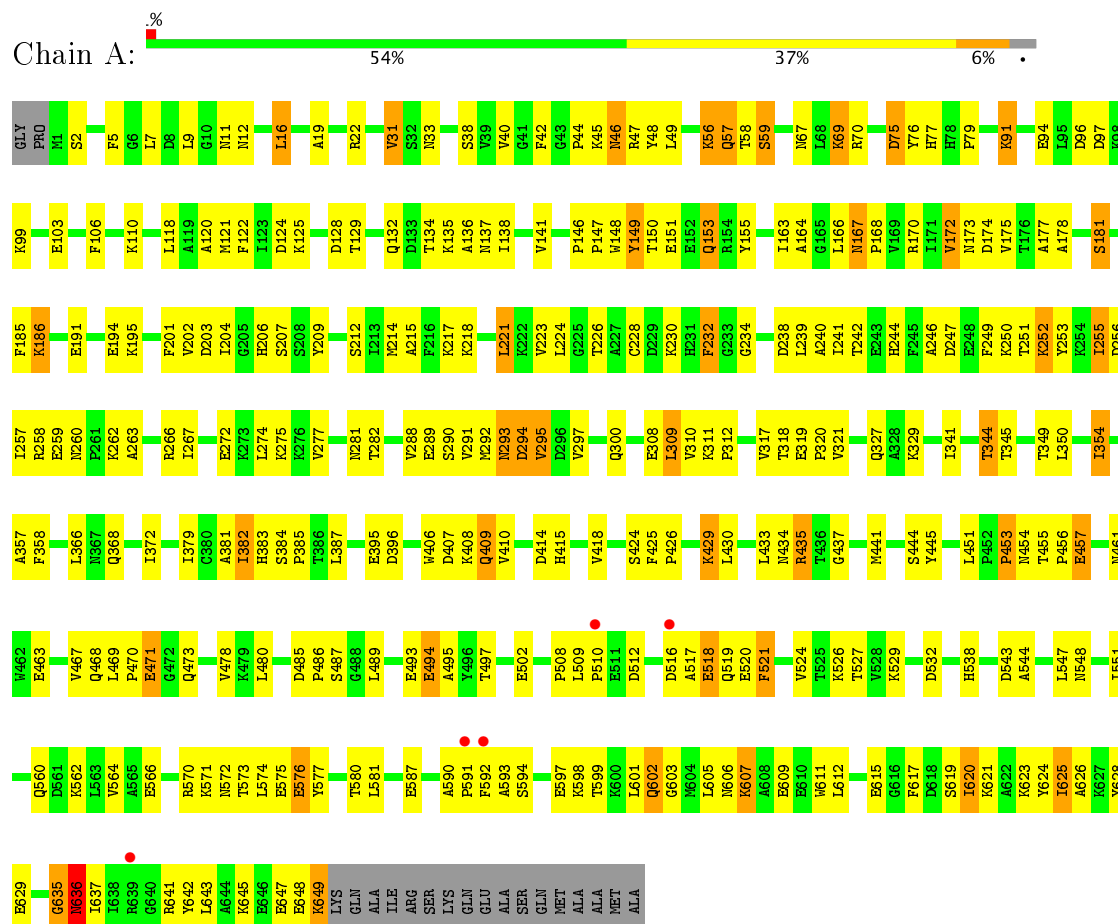
- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	3	Total	Cl	0	0
			3	3		

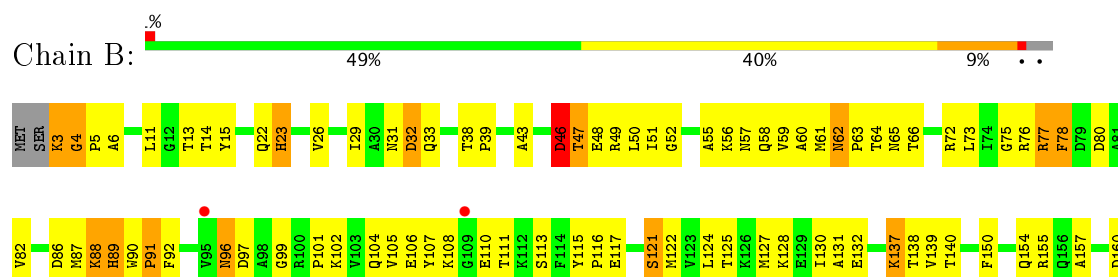
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Heat shock protein homolog SSE1



• Molecule 2: Heat shock cognate



T502	T503	T504	T505	T506	K507	G508	G509	L510	S511	E512	E513	D514	G	R517	K526	A527	E528	D529	E530	K531	Q632	K635	G	S538	K539	N540	S541	L542	E543	S544	Y545	A546	F547	ASN	MET	LYS	TYS	ALA	THR	VAL	GLU	V409	K328	K249	A161																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																					
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K507	G508	T504	N505	D506	P421	T425	F428	T429	S430	T431	S432	D433	N434	Q435	P436	Q437	V438	L439	V442	R447	A448	T449	K451	D452	F459	E460	L461	T462	A463	I464	ASN	A467	P468	R469	T470	V471	P472	T477	I480	T485	V488	V491	T495	G496	K497	K500	T501	K502	K503	K504	K505	K506	K507	K508	K509	K510	K511	K512	K513	K514	K515	K516	K517	K518	K519	K520	K521	K522	K523	K524	K525	K526	K527	K528	K529	K530	K531	K532	K533	K534	K535	K536	K537	K538	K539	K540	K541	K542	K543	K544	K545	K546	K547	K548	K549	K550	K551	K552	K553	K554	K555	K556	K557	K558	K559	K560	K561	K562	K563	K564	K565	K566	K567	K568	K569	K570	K571	K572	K573	K574	K575	K576	K577	K578	K579	K580	K581	K582	K583	K584	K585	K586	K587	K588	K589	K590	K591	K592	K593	K594	K595	K596	K597	K598	K599	K600	K601	K602	K603	K604	K605	K606	K607	K608	K609	K610	K611	K612	K613	K614	K615	K616	K617	K618	K619	K620	K621	K622	K623	K624	K625	K626	K627	K628	K629	K630	K631	K632	K633	K634	K635	K636	K637	K638	K639	K640	K641	K642	K643	K644	K645	K646	K647	K648	K649	K650	K651	K652	K653	K654	K655	K656	K657	K658	K659	K660	K661	K662	K663	K664	K665	K666	K667	K668	K669	K670	K671	K672	K673	K674	K675	K676	K677	K678	K679	K680	K681	K682	K683	K684	K685	K686	K687	K688	K689	K690	K691	K692	K693	K694	K695	K696	K697	K698	K699	K700	K701	K702	K703	K704	K705	K706	K707	K708	K709	K710	K711	K712	K713	K714	K715	K716	K717	K718	K719	K720	K721	K722	K723	K724	K725	K726	K727	K728	K729	K730	K731	K732	K733	K734	K735	K736	K737	K738	K739	K740	K741	K742	K743	K744	K745	K746	K747	K748	K749	K750	K751	K752	K753	K754	K755	K756	K757	K758	K759	K760	K761	K762	K763	K764	K765	K766	K767	K768	K769	K770	K771	K772	K773	K774	K775	K776	K777	K778	K779	K780	K781	K782	K783	K784	K785	K786	K787	K788	K789	K790	K791	K792	K793	K794	K795	K796	K797	K798	K799	K800	K801	K802	K803	K804	K805	K806	K807	K808	K809	K810	K811	K812	K813	K814	K815	K816	K817	K818	K819	K820	K821	K822	K823	K824	K825	K826	K827	K828	K829	K830	K831	K832	K833	K834	K835	K836	K837	K838	K839	K840	K841	K842	K843	K844	K845	K846	K847	K848	K849	K850	K851	K852	K853	K854	K855	K856	K857	K858	K859	K860	K861	K862	K863	K864	K865	K866	K867	K868	K869	K870	K871	K872	K873	K874	K875	K876	K877	K878	K879	K880	K881	K882	K883	K884	K885	K886	K887	K888	K889	K890	K891	K892	K893	K894	K895	K896	K897	K898	K899	K900	K901	K902	K903	K904	K905	K906	K907	K908	K909	K910	K911	K912	K913	K914	K915	K916	K917	K918	K919	K920	K921	K922	K923	K924	K925	K926	K927	K928	K929	K930	K931	K932	K933	K934	K935	K936	K937	K938	K939	K940	K941	K942	K943	K944	K945	K946	K947	K948	K949	K950	K951	K952	K953	K954	K955	K956	K957	K958	K959	K960	K961	K962	K963	K964	K965	K966	K967	K968	K969	K970	K971	K972	K973	K974	K975	K976	K977	K978	K979	K980	K981	K982	K983	K984	K985	K986	K987	K988	K989	K990	K991	K992	K993	K994	K995	K996	K997	K998	K999	K1000																																																																																																																
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	123.53 Å 169.50 Å 87.72 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.38 – 3.12 42.38 – 3.12	Depositor EDS
% Data completeness (in resolution range)	96.5 (42.38-3.12) 96.6 (42.38-3.12)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 3.12 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.224 , 0.283 0.215 , 0.276	Depositor DCC
R_{free} test set	1650 reflections (5.08%)	DCC
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9368	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BEF, SO4, ADP, CL

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	0.56	0/5199	0.70	0/7037
2	B	0.56	1/4242 (0.0%)	0.70	1/5728 (0.0%)
All	All	0.56	1/9441 (0.0%)	0.70	1/12765 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	ARG	CG-CD	5.82	1.66	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	ARG	NE-CZ-NH2	-5.67	117.47	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	420	ILE	Peptide

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	5103	0	5079	245	0
2	B	4182	0	4209	243	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	15	0	0	0	0
4	B	5	0	0	0	0
5	A	4	0	0	0	0
6	A	27	0	12	1	0
6	B	27	0	12	5	0
7	B	3	0	0	2	0
All	All	9368	0	9312	473	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 25.

All (473) 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)
2:B:420:ILE:HG23	2:B:421:PRO:CD	1.75	1.15
1:A:594:SER:HB3	1:A:597:GLU:HG2	1.32	1.11
1:A:601:LEU:O	1:A:603:GLY:HA3	1.53	1.09
1:A:141:VAL:HG21	1:A:166:LEU:HD13	1.40	1.03
2:B:405:THR:HB	2:B:409:VAL:HG23	1.44	0.97
1:A:47:ARG:NH1	1:A:121:MET:HG2	1.80	0.95
1:A:408:LYS:HB2	1:A:414:ASP:HB3	1.48	0.94
2:B:420:ILE:HG23	2:B:421:PRO:HD2	1.48	0.94
1:A:75:ASP:OD1	1:A:99:LYS:HE2	1.70	0.91
2:B:508:GLY:HA2	2:B:509:ARG:HB2	1.52	0.90
2:B:542:LEU:HD12	2:B:543:GLU:H	1.36	0.89
2:B:439:LEU:HB2	2:B:544:SER:HA	1.53	0.89
1:A:594:SER:HB3	1:A:597:GLU:CG	2.03	0.89
1:A:174:ASP:HB2	1:A:372:ILE:HG21	1.56	0.88
1:A:572:ASN:HD21	2:B:300:ALA:H	1.19	0.88
2:B:420:ILE:HG23	2:B:421:PRO:HD3	1.53	0.88
2:B:376:GLN:HE21	2:B:376:GLN:HA	1.39	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:PHE:CD2	1:A:642:TYR:HA	2.12	0.85
1:A:470:PRO:HB2	1:A:473:GLN:HG3	1.58	0.82
1:A:593:ALA:HA	1:A:641:ARG:HH21	1.45	0.82
2:B:258:ARG:HH21	2:B:261:ARG:HH22	1.27	0.82
1:A:575:GLU:HG2	2:B:300:ALA:HB3	1.62	0.82
2:B:110:GLU:HG2	2:B:111:THR:N	1.93	0.81
2:B:110:GLU:HG2	2:B:111:THR:H	1.46	0.81
1:A:244:HIS:HB2	1:A:309:LEU:HD21	1.64	0.80
1:A:434:ASN:C	1:A:435:ARG:HD2	2.02	0.80
2:B:405:THR:HB	2:B:409:VAL:CG2	2.11	0.80
2:B:195:VAL:HG23	2:B:333:ASP:HB2	1.62	0.79
1:A:575:GLU:OE2	2:B:301:ARG:HG3	1.82	0.79
1:A:238:ASP:OD1	1:A:275:LYS:HE2	1.83	0.78
2:B:46:ASP:HA	2:B:108:LYS:HA	1.66	0.77
1:A:602:GLN:HG3	1:A:603:GLY:CA	2.14	0.77
2:B:102:LYS:HE3	2:B:113:SER:OG	1.84	0.77
2:B:237:MET:HE3	2:B:267:CYS:HB3	1.66	0.76
1:A:395:GLU:HB3	1:A:424:SER:HB3	1.68	0.75
1:A:202:VAL:HG11	1:A:354:ILE:HD12	1.67	0.75
2:B:177:THR:HG22	2:B:210:LEU:HD13	1.68	0.75
1:A:350:LEU:O	1:A:354:ILE:HG22	1.86	0.75
2:B:546:ALA:O	2:B:547:PHE:HB2	1.86	0.75
1:A:260:ASN:HB3	1:A:263:ALA:HB3	1.69	0.74
2:B:430:THR:HG21	2:B:472:PRO:HG2	1.69	0.74
1:A:407:ASP:O	1:A:435:ARG:NH2	2.20	0.73
2:B:6:ALA:H	2:B:384:LYS:HE3	1.53	0.73
2:B:340:SER:O	2:B:343:ILE:HG12	1.87	0.73
1:A:2:SER:HB3	1:A:137:ASN:HB3	1.71	0.73
2:B:542:LEU:HD12	2:B:543:GLU:N	2.03	0.72
1:A:636:ASN:H	1:A:636:ASN:ND2	1.87	0.72
2:B:542:LEU:HG	2:B:545:TYR:HB3	1.71	0.72
1:A:147:PRO:HA	1:A:173:ASN:OD1	1.90	0.72
1:A:602:GLN:HG3	1:A:603:GLY:HA3	1.72	0.72
1:A:574:LEU:HD23	1:A:612:LEU:HD11	1.70	0.72
2:B:38:THR:HB	2:B:127:MET:CE	2.19	0.72
2:B:244:GLU:OE2	2:B:295:THR:HG21	1.90	0.72
1:A:209:TYR:CE1	1:A:320:PRO:HG2	2.25	0.71
1:A:76:TYR:CD2	1:A:94:GLU:HB2	2.25	0.71
2:B:435:GLN:HG3	2:B:543:GLU:HB3	1.73	0.71
1:A:426:PRO:HG3	1:A:486:PRO:HA	1.71	0.71
1:A:590:ALA:HB3	1:A:591:PRO:HD3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:THR:HB	2:B:127:MET:HE3	1.72	0.71
2:B:76:ARG:O	2:B:101:PRO:HD3	1.91	0.70
2:B:88:LYS:HE2	2:B:89:HIS:ND1	2.06	0.70
2:B:90:TRP:HB3	2:B:92:PHE:CE2	2.27	0.69
2:B:73:LEU:CD1	2:B:116:PRO:HG3	2.23	0.69
1:A:191:GLU:OE1	1:A:218:LYS:HE3	1.93	0.69
1:A:480:LEU:HD23	1:A:495:ALA:HB2	1.72	0.69
1:A:91:LYS:HD3	1:A:103:GLU:OE1	1.93	0.68
2:B:246:LYS:HG3	2:B:252:ASP:HB2	1.74	0.68
1:A:47:ARG:HH11	1:A:121:MET:HG2	1.55	0.68
2:B:268:GLU:OE1	2:B:272:ARG:HD3	1.93	0.68
2:B:43:ALA:HB2	2:B:66:THR:HG23	1.76	0.68
1:A:444:SER:HB2	1:A:457:GLU:O	1.94	0.68
1:A:434:ASN:O	1:A:435:ARG:HD2	1.94	0.68
1:A:601:LEU:C	1:A:603:GLY:HA3	2.13	0.68
2:B:505:ASN:O	2:B:506:ASP:HB2	1.94	0.68
1:A:194:GLU:O	1:A:217:LYS:HE2	1.94	0.67
1:A:234:GLY:HA2	1:A:344:THR:HG21	1.76	0.67
2:B:64:THR:HA	2:B:91:PRO:O	1.95	0.67
1:A:517:ALA:O	1:A:518:GLU:HB3	1.94	0.67
1:A:575:GLU:HG2	2:B:300:ALA:CB	2.25	0.67
2:B:174:ASN:HB3	2:B:176:PRO:HD2	1.77	0.67
1:A:572:ASN:ND2	2:B:300:ALA:H	1.90	0.67
1:A:560:GLN:O	1:A:564:VAL:HG23	1.95	0.67
1:A:518:GLU:HG3	1:A:518:GLU:O	1.94	0.66
1:A:645:LYS:O	1:A:649:LYS:HB2	1.95	0.66
1:A:611:TRP:HE3	1:A:612:LEU:HD12	1.57	0.66
2:B:51:ILE:HD13	2:B:122:MET:O	1.96	0.66
1:A:574:LEU:CD2	1:A:612:LEU:HD11	2.25	0.66
1:A:456:PRO:O	1:A:457:GLU:CB	2.44	0.66
2:B:532:GLN:HA	2:B:535:LYS:HD3	1.78	0.66
2:B:77:ARG:O	2:B:80:ASP:HB2	1.94	0.66
1:A:118:LEU:HA	1:A:121:MET:HE3	1.77	0.65
2:B:117:GLU:O	2:B:121:SER:HB3	1.96	0.65
2:B:11:LEU:HD13	2:B:124:LEU:HD11	1.78	0.65
1:A:341:ILE:HD12	1:A:372:ILE:HD11	1.79	0.65
2:B:395:ASP:HB2	2:B:420:ILE:HG21	1.77	0.65
1:A:385:PRO:HG3	2:B:512:LYS:N	2.11	0.65
2:B:299:ARG:O	2:B:303:GLU:HG3	1.96	0.65
1:A:445:TYR:CD1	1:A:451:LEU:HD21	2.32	0.64
2:B:132:GLU:HG3	2:B:139:VAL:HG23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:LEU:HD13	2:B:116:PRO:HG3	1.79	0.64
2:B:539:LYS:HG3	2:B:539:LYS:O	1.97	0.64
2:B:376:GLN:NE2	2:B:376:GLN:HA	2.13	0.63
1:A:445:TYR:CE1	1:A:451:LEU:HD21	2.32	0.63
1:A:547:LEU:O	1:A:551:ILE:HG13	1.99	0.62
1:A:253:TYR:HB3	1:A:255:ILE:HD13	1.82	0.62
2:B:50:LEU:O	2:B:55:ALA:HB2	1.99	0.62
2:B:246:LYS:HA	2:B:251:LYS:O	1.99	0.62
2:B:191:ALA:HB3	7:B:555:CL:CL	2.37	0.61
2:B:90:TRP:HB3	2:B:92:PHE:CZ	2.35	0.61
2:B:78:PHE:CD2	2:B:96:ASN:HB2	2.36	0.61
1:A:562:LYS:O	1:A:566:GLU:HB2	1.99	0.61
2:B:86:ASP:O	2:B:88:LYS:N	2.34	0.61
2:B:73:LEU:HD23	2:B:90:TRP:CZ3	2.36	0.61
1:A:594:SER:CB	1:A:597:GLU:HG2	2.21	0.60
2:B:279:GLN:HG2	2:B:280:ALA:H	1.66	0.60
2:B:531:LYS:HD3	2:B:531:LYS:O	2.01	0.60
1:A:636:ASN:H	1:A:636:ASN:HD22	1.48	0.60
1:A:435:ARG:HG2	1:A:478:VAL:HG22	1.83	0.60
1:A:625:ILE:O	1:A:629:GLU:HG2	2.02	0.60
2:B:467:ALA:HB1	2:B:468:PRO:CD	2.32	0.60
1:A:19:ALA:HB1	2:B:393:LEU:HD11	1.83	0.60
1:A:310:VAL:C	1:A:312:PRO:HD2	2.22	0.60
1:A:529:LYS:HE2	1:A:532:ASP:OD2	2.01	0.60
2:B:102:LYS:HD2	2:B:115:TYR:CE1	2.37	0.60
2:B:11:LEU:HD13	2:B:124:LEU:CD1	2.31	0.60
2:B:96:ASN:HD21	2:B:99:GLY:H	1.50	0.60
1:A:385:PRO:HG3	2:B:512:LYS:H	1.67	0.59
2:B:430:THR:CG2	2:B:472:PRO:HG2	2.32	0.59
1:A:519:GLN:HE21	1:A:520:GLU:N	2.00	0.59
1:A:203:ASP:HA	1:A:341:ILE:O	2.02	0.59
2:B:78:PHE:C	2:B:78:PHE:CD1	2.75	0.59
1:A:575:GLU:OE1	2:B:298:THR:HG21	2.03	0.59
2:B:508:GLY:CA	2:B:509:ARG:HB2	2.29	0.59
1:A:478:VAL:HG12	1:A:497:THR:CG2	2.33	0.59
1:A:291:VAL:HG23	1:A:292:MET:N	2.18	0.58
1:A:12:ASN:HB2	1:A:206:HIS:CG	2.38	0.58
2:B:439:LEU:CB	2:B:544:SER:HA	2.31	0.58
2:B:73:LEU:HD23	2:B:90:TRP:CH2	2.38	0.58
2:B:60:ALA:O	2:B:61:MET:HG3	2.02	0.58
2:B:110:GLU:CG	2:B:111:THR:H	2.11	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ASN:OD1	1:A:67:ASN:HA	2.03	0.58
2:B:117:GLU:HG2	2:B:157:ALA:HB1	1.84	0.58
2:B:248:LYS:C	2:B:249:HIS:CD2	2.77	0.58
2:B:539:LYS:CG	2:B:539:LYS:O	2.52	0.58
1:A:581:LEU:HD23	1:A:605:LEU:HD11	1.86	0.57
1:A:317:VAL:O	1:A:320:PRO:HD2	2.04	0.57
1:A:46:ASN:HB3	1:A:564:VAL:HG21	1.85	0.57
1:A:70:ARG:NH2	1:A:230:LYS:O	2.34	0.57
1:A:253:TYR:HB3	1:A:255:ILE:CD1	2.35	0.57
1:A:344:THR:HG23	6:A:672:ADP:H1'	1.86	0.57
1:A:221:LEU:C	1:A:221:LEU:HD12	2.25	0.57
1:A:456:PRO:O	1:A:457:GLU:HB3	2.03	0.57
2:B:132:GLU:HG2	2:B:138:THR:HA	1.85	0.57
2:B:185:LEU:CD1	2:B:195:VAL:HG21	2.33	0.57
2:B:343:ILE:CD1	6:B:560:ADP:H2	2.18	0.57
2:B:62:ASN:N	2:B:63:PRO:CD	2.67	0.57
1:A:42:PHE:HB3	1:A:106:PHE:HB2	1.86	0.57
1:A:599:THR:HG22	1:A:599:THR:O	2.05	0.57
2:B:185:LEU:C	2:B:187:LYS:H	2.08	0.56
2:B:96:ASN:HD22	2:B:97:ASP:N	2.03	0.56
1:A:91:LYS:HG2	1:A:103:GLU:HB3	1.85	0.56
1:A:478:VAL:HG12	1:A:497:THR:HG22	1.86	0.56
1:A:621:LYS:O	1:A:625:ILE:HG12	2.05	0.56
1:A:426:PRO:HG3	1:A:486:PRO:CA	2.36	0.56
1:A:262:LYS:O	1:A:266:ARG:HG3	2.06	0.56
1:A:396:ASP:HB3	1:A:425:PHE:CE2	2.39	0.56
1:A:572:ASN:HD21	2:B:300:ALA:N	1.96	0.56
1:A:469:LEU:HD12	1:A:469:LEU:N	2.20	0.56
1:A:590:ALA:HA	1:A:598:LYS:NZ	2.21	0.56
1:A:150:THR:H	1:A:153:GLN:HG3	1.71	0.56
1:A:406:TRP:CE2	1:A:433:LEU:HD21	2.42	0.55
2:B:405:THR:HG23	2:B:540:ASN:H	1.72	0.55
1:A:451:LEU:CD2	1:A:455:THR:HG21	2.36	0.55
2:B:78:PHE:C	2:B:78:PHE:HD1	2.10	0.55
2:B:430:THR:HG22	2:B:472:PRO:HD2	1.88	0.55
1:A:601:LEU:O	1:A:602:GLN:CG	2.55	0.55
1:A:266:ARG:NH1	1:A:289:GLU:O	2.37	0.54
1:A:76:TYR:CG	1:A:94:GLU:HB2	2.42	0.54
2:B:395:ASP:CB	2:B:420:ILE:HG21	2.36	0.54
1:A:509:LEU:N	1:A:510:PRO:HD3	2.23	0.54
1:A:641:ARG:O	1:A:645:LYS:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:437:GLY:O	2:B:543:GLU:HA	2.07	0.54
2:B:248:LYS:O	2:B:249:HIS:CD2	2.61	0.54
2:B:286:SER:N	2:B:292:ASP:OD2	2.34	0.54
2:B:460:GLU:HG2	2:B:462:THR:CG2	2.38	0.54
1:A:137:ASN:O	1:A:138:ILE:HD13	2.08	0.54
2:B:3:LYS:HB2	2:B:137:LYS:HE3	1.88	0.54
2:B:436:PRO:O	2:B:464:ILE:HG13	2.08	0.54
1:A:246:ALA:HB2	1:A:257:ILE:HD11	1.90	0.54
1:A:451:LEU:HD22	1:A:455:THR:HG21	1.89	0.54
2:B:338:GLY:HA2	6:B:560:ADP:O2A	2.08	0.54
2:B:429:THR:CG2	2:B:540:ASN:HB3	2.38	0.54
1:A:290:SER:HA	1:A:295:VAL:O	2.07	0.54
1:A:134:THR:C	1:A:136:ALA:H	2.11	0.53
1:A:257:ILE:C	1:A:259:GLU:H	2.10	0.53
1:A:150:THR:H	1:A:153:GLN:CG	2.21	0.53
1:A:433:LEU:HB3	1:A:435:ARG:HD3	1.91	0.53
2:B:351:GLN:HB2	2:B:359:LEU:HD11	1.90	0.53
1:A:385:PRO:CD	2:B:509:ARG:HH22	2.20	0.53
1:A:571:LYS:HE2	1:A:617:PHE:O	2.07	0.53
1:A:141:VAL:CG2	1:A:166:LEU:HD13	2.25	0.53
1:A:408:LYS:HG2	1:A:408:LYS:O	2.06	0.53
1:A:636:ASN:N	1:A:636:ASN:ND2	2.51	0.53
2:B:86:ASP:C	2:B:88:LYS:H	2.12	0.53
1:A:384:SER:CB	1:A:387:LEU:HD12	2.39	0.53
1:A:623:LYS:HA	1:A:626:ALA:HB3	1.91	0.53
2:B:31:ASN:C	2:B:33:GLN:H	2.12	0.53
2:B:438:VAL:HG23	2:B:461:LEU:HB3	1.91	0.53
2:B:429:THR:HG22	2:B:540:ASN:HB3	1.90	0.53
2:B:183:TYR:OH	2:B:361:LYS:HA	2.09	0.52
1:A:311:LYS:N	1:A:312:PRO:CD	2.73	0.52
1:A:643:LEU:O	1:A:647:GLU:HB2	2.08	0.52
2:B:221:SER:OG	2:B:324:ALA:HB2	2.09	0.52
2:B:29:ILE:HD13	2:B:131:ALA:HA	1.91	0.52
2:B:240:HIS:CB	2:B:305:LEU:HD21	2.39	0.52
2:B:229:GLY:O	2:B:230:GLY:C	2.47	0.52
2:B:240:HIS:O	2:B:243:ALA:HB3	2.10	0.52
1:A:201:PHE:HE1	1:A:366:LEU:HD11	1.73	0.52
2:B:90:TRP:C	2:B:92:PHE:H	2.12	0.52
1:A:91:LYS:HD3	1:A:103:GLU:CD	2.30	0.52
1:A:150:THR:OG1	1:A:153:GLN:HG2	2.10	0.52
1:A:260:ASN:HB3	1:A:263:ALA:CB	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:368:ALA:O	2:B:371:TYR:HB3	2.10	0.52
1:A:170:ARG:HE	1:A:383:HIS:HE1	1.57	0.52
1:A:635:GLY:O	1:A:636:ASN:C	2.48	0.52
1:A:341:ILE:HA	1:A:368:GLN:HB2	1.91	0.51
2:B:106:GLU:O	2:B:106:GLU:HG3	2.08	0.51
2:B:253:ILE:O	2:B:255:GLU:N	2.43	0.51
2:B:96:ASN:HD21	2:B:99:GLY:N	2.07	0.51
1:A:256:ASP:HB3	1:A:259:GLU:CG	2.40	0.51
1:A:7:LEU:HD21	1:A:9:LEU:HD12	1.92	0.51
2:B:185:LEU:HD12	2:B:195:VAL:HG21	1.91	0.51
2:B:279:GLN:HG2	2:B:280:ALA:N	2.26	0.51
2:B:75:GLY:HA3	2:B:154:GLN:HA	1.93	0.51
2:B:86:ASP:HB3	2:B:90:TRP:CH2	2.45	0.51
2:B:248:LYS:HB3	2:B:249:HIS:CD2	2.45	0.51
2:B:405:THR:HG22	2:B:406:ALA:N	2.25	0.51
2:B:503:ILE:C	2:B:505:ASN:H	2.14	0.51
2:B:117:GLU:CG	2:B:157:ALA:HB1	2.41	0.51
1:A:649:LYS:HB3	1:A:649:LYS:NZ	2.26	0.50
1:A:214:MET:HG2	1:A:223:VAL:HG22	1.92	0.50
2:B:315:ASP:HB2	2:B:316:PRO:HD3	1.93	0.50
2:B:238:VAL:O	2:B:242:ILE:HD12	2.10	0.50
1:A:146:PRO:HB2	1:A:148:TRP:CD1	2.46	0.50
1:A:291:VAL:CG2	1:A:292:MET:H	2.24	0.50
2:B:197:ILE:N	2:B:197:ILE:HD13	2.27	0.50
2:B:430:THR:CG2	2:B:472:PRO:HD2	2.42	0.50
2:B:542:LEU:HD21	2:B:545:TYR:HD1	1.77	0.50
1:A:291:VAL:CG2	1:A:292:MET:N	2.75	0.50
1:A:470:PRO:CB	1:A:473:GLN:HG3	2.35	0.50
2:B:22:GLN:O	2:B:23:HIS:HB2	2.12	0.50
2:B:343:ILE:HD13	6:B:560:ADP:H2	1.76	0.50
1:A:212:SER:HB2	1:A:226:THR:OG1	2.12	0.50
1:A:318:THR:HG22	1:A:357:ALA:HB2	1.93	0.50
1:A:379:ILE:O	1:A:382:ILE:HB	2.12	0.50
2:B:6:ALA:HB1	2:B:377:ALA:HB1	1.93	0.50
1:A:174:ASP:HB2	1:A:372:ILE:CG2	2.34	0.49
1:A:620:ILE:HD11	1:A:623:LYS:HG2	1.94	0.49
1:A:70:ARG:NH1	1:A:207:SER:OG	2.44	0.49
2:B:106:GLU:HA	2:B:110:GLU:O	2.11	0.49
2:B:132:GLU:CG	2:B:139:VAL:HG23	2.43	0.49
2:B:324:ALA:O	2:B:326:LEU:HG	2.12	0.49
2:B:375:VAL:O	2:B:378:ALA:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:72:ARG:HH12	2:B:226:THR:HG22	1.76	0.49
1:A:544:ALA:O	1:A:548:ASN:ND2	2.46	0.49
2:B:121:SER:HB2	2:B:161:ALA:O	2.12	0.49
2:B:298:THR:CG2	2:B:301:ARG:H	2.24	0.49
1:A:292:MET:O	1:A:294:ASP:N	2.46	0.49
2:B:471:VAL:HB	2:B:472:PRO:HD3	1.94	0.49
1:A:204:ILE:HD13	1:A:345:THR:HG22	1.93	0.48
1:A:128:ASP:O	1:A:129:THR:C	2.52	0.48
2:B:286:SER:HA	2:B:291:ILE:O	2.13	0.48
1:A:9:LEU:O	1:A:69:LYS:HE2	2.14	0.48
2:B:102:LYS:HD2	2:B:115:TYR:CZ	2.49	0.48
2:B:62:ASN:H	2:B:63:PRO:CD	2.25	0.48
1:A:256:ASP:O	1:A:259:GLU:CG	2.62	0.48
1:A:451:LEU:N	1:A:451:LEU:HD12	2.29	0.48
1:A:607:LYS:O	1:A:611:TRP:HB2	2.13	0.48
2:B:32:ASP:OD2	2:B:32:ASP:N	2.46	0.48
1:A:2:SER:HB2	1:A:137:ASN:O	2.12	0.48
1:A:56:LYS:O	1:A:58:THR:N	2.47	0.48
1:A:150:THR:N	1:A:153:GLN:HG3	2.29	0.48
2:B:238:VAL:HG12	2:B:242:ILE:HD11	1.96	0.48
2:B:26:VAL:HB	2:B:371:TYR:CE2	2.48	0.48
2:B:460:GLU:HG2	2:B:462:THR:HG23	1.96	0.48
1:A:134:THR:C	1:A:136:ALA:N	2.66	0.48
1:A:75:ASP:HA	1:A:99:LYS:HD3	1.96	0.48
2:B:110:GLU:CG	2:B:111:THR:N	2.66	0.48
2:B:198:PHE:CD1	2:B:198:PHE:O	2.67	0.47
2:B:467:ALA:HB1	2:B:468:PRO:HD3	1.97	0.47
1:A:385:PRO:HD2	2:B:509:ARG:HH22	1.79	0.47
2:B:38:THR:HB	2:B:127:MET:HE1	1.96	0.47
2:B:500:LYS:HG3	2:B:501:ILE:N	2.29	0.47
1:A:601:LEU:O	1:A:602:GLN:HG2	2.14	0.47
2:B:364:ASN:HA	2:B:365:PRO:HD2	1.74	0.47
2:B:228:LEU:HD22	2:B:229:GLY:N	2.30	0.47
2:B:425:THR:HG23	2:B:477:THR:OG1	2.14	0.47
1:A:396:ASP:O	1:A:424:SER:HA	2.15	0.47
1:A:623:LYS:HA	1:A:626:ALA:CB	2.44	0.47
1:A:38:SER:HA	1:A:122:PHE:CE1	2.50	0.47
1:A:178:ALA:O	1:A:181:SER:HB2	2.14	0.47
2:B:298:THR:HG22	2:B:301:ARG:HB2	1.97	0.47
1:A:485:ASP:HB2	1:A:486:PRO:CD	2.45	0.47
1:A:461:ASN:ND2	1:A:538:HIS:HD2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:442:VAL:HG21	2:B:488:VAL:HG21	1.97	0.47
1:A:97:ASP:OD1	1:A:99:LYS:HB2	2.15	0.46
1:A:59:SER:OG	2:B:283:GLU:OE1	2.28	0.46
2:B:543:GLU:O	2:B:545:TYR:N	2.49	0.46
2:B:107:TYR:O	2:B:108:LYS:HB2	2.15	0.46
2:B:31:ASN:HB3	2:B:130:ILE:HD13	1.97	0.46
2:B:249:HIS:ND1	2:B:291:ILE:HG21	2.31	0.46
1:A:288:VAL:H	1:A:297:VAL:HG23	1.81	0.46
1:A:327:GLN:C	1:A:329:LYS:H	2.18	0.46
2:B:233:PHE:CD1	2:B:310:PHE:HE1	2.34	0.46
2:B:328:LYS:HE3	2:B:353:PHE:O	2.16	0.46
2:B:531:LYS:CD	2:B:531:LYS:O	2.64	0.46
1:A:132:GLN:O	1:A:135:LYS:HE3	2.16	0.46
1:A:256:ASP:O	1:A:259:GLU:HG2	2.16	0.46
1:A:281:ASN:HD21	2:B:57:ASN:HB2	1.80	0.46
1:A:592:PHE:CE2	1:A:642:TYR:HA	2.49	0.46
2:B:301:ARG:O	2:B:305:LEU:CD1	2.64	0.46
2:B:339:GLY:N	6:B:560:ADP:O2A	2.45	0.46
2:B:303:GLU:OE2	2:B:345:LYS:HB2	2.16	0.46
2:B:420:ILE:CG2	2:B:421:PRO:CD	2.69	0.45
2:B:191:ALA:CB	7:B:555:CL:CL	3.01	0.45
2:B:200:LEU:HD11	2:B:228:LEU:HD13	1.99	0.45
2:B:526:LYS:O	2:B:530:GLU:HB2	2.16	0.45
2:B:339:GLY:O	2:B:342:ARG:HG3	2.17	0.45
2:B:49:ARG:O	2:B:50:LEU:HD23	2.15	0.45
1:A:174:ASP:OD1	1:A:175:VAL:N	2.45	0.45
1:A:232:PHE:C	1:A:232:PHE:CD2	2.90	0.45
1:A:204:ILE:HG13	1:A:209:TYR:CD2	2.51	0.45
1:A:606:ASN:O	1:A:609:GLU:HB3	2.17	0.45
2:B:436:PRO:HG2	2:B:437:GLY:H	1.81	0.45
1:A:602:GLN:HG3	1:A:603:GLY:HA2	1.93	0.45
1:A:487:SER:HB2	1:A:489:LEU:HG	1.98	0.45
2:B:480:ILE:HA	2:B:485:ILE:O	2.17	0.45
1:A:16:LEU:N	1:A:16:LEU:CD1	2.79	0.45
1:A:172:VAL:HG21	1:A:379:ILE:CD1	2.46	0.45
2:B:459:PHE:CE1	2:B:501:ILE:HG22	2.52	0.45
2:B:249:HIS:C	2:B:251:LYS:H	2.20	0.44
1:A:291:VAL:HG23	1:A:292:MET:H	1.79	0.44
2:B:392:LEU:C	2:B:392:LEU:HD12	2.38	0.44
1:A:203:ASP:C	1:A:203:ASP:OD2	2.56	0.44
1:A:381:ALA:O	1:A:382:ILE:C	2.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:VAL:HG22	1:A:49:LEU:HD22	2.00	0.44
2:B:508:GLY:HA2	2:B:509:ARG:CB	2.34	0.44
1:A:31:VAL:CG2	1:A:33:ASN:ND2	2.80	0.44
1:A:418:VAL:O	1:A:429:LYS:HE3	2.17	0.44
1:A:577:TYR:HA	1:A:580:THR:HG22	2.00	0.44
2:B:279:GLN:NE2	2:B:296:SER:HB2	2.33	0.44
2:B:449:MET:O	2:B:451:LYS:N	2.51	0.44
1:A:249:PHE:O	1:A:255:ILE:O	2.35	0.44
1:A:406:TRP:O	1:A:414:ASP:HB2	2.18	0.44
2:B:46:ASP:CA	2:B:108:LYS:HA	2.43	0.44
2:B:256:ASN:HB3	2:B:259:ALA:HB3	2.00	0.44
1:A:56:LYS:O	1:A:57:GLN:C	2.56	0.44
1:A:48:TYR:CD2	1:A:56:LYS:HG2	2.53	0.44
2:B:469:ARG:HG2	2:B:469:ARG:O	2.18	0.44
2:B:542:LEU:HG	2:B:545:TYR:CB	2.42	0.44
1:A:310:VAL:C	1:A:312:PRO:CD	2.86	0.43
1:A:49:LEU:HD23	1:A:49:LEU:HA	1.74	0.43
2:B:405:THR:CG2	2:B:406:ALA:N	2.81	0.43
2:B:435:GLN:CG	2:B:543:GLU:HB3	2.45	0.43
1:A:146:PRO:HG2	1:A:149:TYR:CD1	2.53	0.43
2:B:104:GLN:HG3	2:B:113:SER:HB3	2.00	0.43
1:A:110:LYS:HA	1:A:110:LYS:HD3	1.80	0.43
1:A:167:ASN:HA	1:A:168:PRO:HD3	1.83	0.43
1:A:174:ASP:O	1:A:177:ALA:N	2.50	0.43
1:A:560:GLN:O	1:A:560:GLN:HG2	2.17	0.43
1:A:573:THR:HG22	1:A:628:TYR:CE1	2.54	0.43
1:A:647:GLU:HB3	1:A:648:GLU:OE2	2.18	0.43
2:B:174:ASN:HB2	2:B:177:THR:OG1	2.18	0.43
1:A:151:GLU:O	1:A:155:TYR:HD1	2.01	0.43
2:B:505:ASN:O	2:B:506:ASP:CB	2.64	0.43
1:A:135:LYS:HE2	1:A:135:LYS:HA	1.99	0.43
1:A:239:LEU:O	1:A:240:ALA:C	2.57	0.43
1:A:406:TRP:HB3	1:A:441:MET:HG2	2.01	0.43
2:B:185:LEU:C	2:B:187:LYS:N	2.72	0.43
2:B:511:SER:O	2:B:514:ASP:N	2.51	0.43
1:A:469:LEU:N	1:A:469:LEU:CD1	2.81	0.43
2:B:178:ALA:O	2:B:372:GLY:HA3	2.19	0.43
2:B:510:LEU:HD22	2:B:514:ASP:HB3	2.01	0.43
1:A:247:ASP:O	1:A:250:LYS:HB3	2.18	0.43
1:A:453:PRO:O	1:A:454:ASN:HB2	2.19	0.43
1:A:521:PHE:CD1	1:A:521:PHE:N	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:PHE:O	1:A:186:LYS:C	2.57	0.43
1:A:425:PHE:HA	1:A:426:PRO:C	2.40	0.43
2:B:240:HIS:HB2	2:B:305:LEU:HD21	2.01	0.43
1:A:463:GLU:OE2	1:A:538:HIS:NE2	2.33	0.42
2:B:319:LYS:O	2:B:319:LYS:HG3	2.18	0.42
2:B:301:ARG:O	2:B:305:LEU:HD12	2.19	0.42
2:B:343:ILE:HD11	6:B:560:ADP:H2	1.84	0.42
2:B:59:VAL:O	2:B:60:ALA:HB3	2.19	0.42
1:A:22:ARG:HH11	2:B:394:LEU:HD12	1.84	0.42
1:A:435:ARG:HG2	1:A:478:VAL:CG2	2.49	0.42
2:B:181:ILE:O	2:B:184:GLY:N	2.47	0.42
2:B:31:ASN:O	2:B:33:GLN:N	2.52	0.42
2:B:251:LYS:HA	2:B:251:LYS:HD3	1.89	0.42
2:B:309:LEU:HD23	2:B:309:LEU:HA	1.80	0.42
2:B:403:ILE:HD11	2:B:428:PHE:CZ	2.54	0.42
1:A:120:ALA:O	1:A:164:ALA:HB2	2.20	0.42
2:B:238:VAL:HG12	2:B:242:ILE:CD1	2.49	0.42
2:B:459:PHE:CD1	2:B:501:ILE:HG22	2.55	0.42
2:B:513:GLU:HG2	2:B:517:ARG:NH2	2.34	0.42
2:B:543:GLU:O	2:B:544:SER:C	2.58	0.42
1:A:395:GLU:HB3	1:A:424:SER:CB	2.44	0.42
1:A:576:GLU:O	1:A:580:THR:HG22	2.19	0.42
1:A:249:PHE:N	1:A:249:PHE:CD1	2.86	0.42
2:B:237:MET:HE1	2:B:271:LYS:HB2	2.01	0.42
2:B:238:VAL:O	2:B:239:ASN:C	2.58	0.42
1:A:564:VAL:O	1:A:564:VAL:HG12	2.20	0.42
2:B:237:MET:CE	2:B:267:CYS:HB3	2.42	0.42
2:B:5:PRO:HB3	2:B:384:LYS:CE	2.50	0.42
2:B:505:ASN:HB3	2:B:507:LYS:HD3	2.01	0.42
2:B:86:ASP:C	2:B:88:LYS:N	2.72	0.42
1:A:251:THR:HG22	1:A:252:LYS:N	2.35	0.42
2:B:65:ASN:OD1	2:B:106:GLU:HB3	2.20	0.42
1:A:274:LEU:O	1:A:277:VAL:HB	2.20	0.41
1:A:414:ASP:O	1:A:415:HIS:HB3	2.20	0.41
1:A:437:GLY:HA2	1:A:467:VAL:HG11	2.02	0.41
1:A:46:ASN:N	1:A:46:ASN:HD22	2.18	0.41
1:A:602:GLN:CG	1:A:603:GLY:HA3	2.45	0.41
1:A:77:HIS:CD2	1:A:94:GLU:OE1	2.73	0.41
2:B:291:ILE:HG22	2:B:292:ASP:N	2.35	0.41
2:B:78:PHE:CE2	2:B:96:ASN:HB2	2.55	0.41
1:A:571:LYS:HA	1:A:624:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:GLU:CD	2:B:272:ARG:HH11	2.23	0.41
2:B:495:THR:OG1	2:B:497:LYS:HG2	2.20	0.41
1:A:103:GLU:OE2	1:A:110:LYS:HD2	2.20	0.41
1:A:409:GLN:HG3	1:A:435:ARG:NH2	2.33	0.41
2:B:336:LEU:HD11	2:B:359:LEU:HD22	2.03	0.41
2:B:150:PHE:O	2:B:155:ARG:NH2	2.51	0.41
2:B:193:ARG:O	2:B:211:THR:HA	2.20	0.41
1:A:215:ALA:HB2	1:A:224:LEU:HD11	2.02	0.41
2:B:39:PRO:O	2:B:52:GLY:HA2	2.21	0.41
2:B:56:LYS:O	2:B:59:VAL:HG12	2.20	0.41
1:A:120:ALA:HB1	1:A:163:ILE:CG2	2.51	0.41
1:A:45:LYS:O	1:A:564:VAL:HG21	2.20	0.41
1:A:502:GLU:HA	1:A:524:VAL:O	2.20	0.41
1:A:623:LYS:HA	1:A:623:LYS:HD3	1.74	0.41
1:A:203:ASP:HB2	1:A:341:ILE:HG13	2.03	0.41
1:A:252:LYS:HG3	1:A:252:LYS:O	2.21	0.41
2:B:15:TYR:CE2	2:B:39:PRO:HG3	2.56	0.41
2:B:543:GLU:C	2:B:545:TYR:N	2.73	0.41
1:A:241:ILE:O	1:A:242:THR:C	2.58	0.41
1:A:251:THR:O	1:A:253:TYR:N	2.52	0.41
1:A:251:THR:C	1:A:253:TYR:H	2.24	0.41
1:A:321:VAL:HG22	1:A:358:PHE:CE2	2.56	0.41
1:A:350:LEU:HD12	1:A:350:LEU:O	2.20	0.41
1:A:526:LYS:HA	1:A:526:LYS:HD3	1.74	0.41
2:B:125:THR:O	2:B:128:LYS:HB3	2.21	0.41
2:B:459:PHE:CD1	2:B:501:ILE:CG2	3.03	0.41
2:B:508:GLY:CA	2:B:509:ARG:CB	2.95	0.41
1:A:611:TRP:CE2	1:A:615:GLU:O	2.75	0.41
2:B:160:ASP:C	2:B:164:ILE:HD12	2.42	0.41
2:B:321:LEU:HD23	2:B:321:LEU:HA	1.74	0.41
1:A:516:ASP:O	1:A:517:ALA:HB2	2.21	0.40
2:B:198:PHE:O	2:B:198:PHE:HD1	2.04	0.40
1:A:125:LYS:O	1:A:128:ASP:HB3	2.20	0.40
1:A:194:GLU:O	1:A:217:LYS:CE	2.65	0.40
1:A:267:ILE:HD13	1:A:288:VAL:HG21	2.03	0.40
1:A:570:ARG:C	1:A:572:ASN:N	2.74	0.40
2:B:419:THR:O	2:B:420:ILE:O	2.40	0.40
2:B:447:ARG:HG3	2:B:452:ASP:HB3	2.03	0.40
1:A:493:GLU:O	1:A:494:GLU:HB2	2.21	0.40
2:B:302:PHE:O	2:B:306:ASN:ND2	2.55	0.40
2:B:343:ILE:HB	2:B:346:ILE:HB	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:GLY:HA2	2:B:5:PRO:HD3	1.78	0.40
1:A:12:ASN:HB2	1:A:206:HIS:CB	2.52	0.40
1:A:571:LYS:O	1:A:571:LYS:HG2	2.20	0.40
2:B:194:ASN:HB2	2:B:330:GLN:O	2.21	0.40
2:B:354:PHE:O	2:B:355:ASN:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	647/668 (97%)	546 (84%)	80 (12%)	21 (3%)	5	26
2	B	536/554 (97%)	442 (82%)	67 (12%)	27 (5%)	2	16
All	All	1183/1222 (97%)	988 (84%)	147 (12%)	48 (4%)	3	19

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	293	ASN
1	A	457	GLU
1	A	471	GLU
1	A	636	ASN
1	A	637	ILE
2	B	46	ASP
2	B	190	GLY
2	B	230	GLY
2	B	420	ILE
2	B	421	PRO
2	B	543	GLU
1	A	57	GLN
1	A	252	LYS

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Mol	Chain	Res	Type
1	A	508	PRO
1	A	518	GLU
1	A	635	GLY
2	B	62	ASN
2	B	186	ASP
2	B	191	ALA
2	B	254	SER
2	B	469	ARG
2	B	506	ASP
2	B	508	GLY
2	B	538	SER
2	B	23	HIS
2	B	32	ASP
2	B	87	MET
2	B	450	THR
2	B	504	THR
2	B	507	LYS
1	A	44	PRO
1	A	258	ARG
1	A	409	GLN
1	A	602	GLN
2	B	47	THR
2	B	305	LEU
1	A	494	GLU
1	A	619	SER
2	B	203	GLY
2	B	378	ALA
2	B	532	GLN
1	A	56	LYS
1	A	294	ASP
1	A	453	PRO
2	B	4	GLY
2	B	91	PRO
1	A	79	PRO
1	A	382	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	560/573 (98%)	511 (91%)	49 (9%)	12	42
2	B	455/468 (97%)	403 (89%)	52 (11%)	7	27
All	All	1015/1041 (98%)	914 (90%)	101 (10%)	9	33

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	PHE
1	A	16	LEU
1	A	31	VAL
1	A	46	ASN
1	A	59	SER
1	A	69	LYS
1	A	75	ASP
1	A	91	LYS
1	A	96	ASP
1	A	124	ASP
1	A	149	TYR
1	A	153	GLN
1	A	167	ASN
1	A	172	VAL
1	A	181	SER
1	A	186	LYS
1	A	195	LYS
1	A	221	LEU
1	A	228	CYS
1	A	232	PHE
1	A	255	ILE
1	A	272	GLU
1	A	282	THR
1	A	293	ASN
1	A	295	VAL
1	A	300	GLN
1	A	308	GLU
1	A	309	LEU
1	A	319	GLU
1	A	344	THR
1	A	349	THR
1	A	354	ILE
1	A	410	VAL
1	A	429	LYS

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Mol	Chain	Res	Type
1	A	430	LEU
1	A	435	ARG
1	A	468	GLN
1	A	471	GLU
1	A	512	ASP
1	A	521	PHE
1	A	527	THR
1	A	543	ASP
1	A	576	GLU
1	A	587	GLU
1	A	607	LYS
1	A	620	ILE
1	A	625	ILE
1	A	636	ASN
1	A	649	LYS
2	B	3	LYS
2	B	13	THR
2	B	14	THR
2	B	46	ASP
2	B	47	THR
2	B	48	GLU
2	B	58	GLN
2	B	77	ARG
2	B	78	PHE
2	B	82	VAL
2	B	88	LYS
2	B	89	HIS
2	B	96	ASN
2	B	105	VAL
2	B	121	SER
2	B	137	LYS
2	B	140	THR
2	B	173	ILE
2	B	193	ARG
2	B	211	THR
2	B	212	ILE
2	B	222	THR
2	B	226	THR
2	B	228	LEU
2	B	250	LYS
2	B	278	THR
2	B	285	ASP

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Mol	Chain	Res	Type
2	B	298	THR
2	B	314	LEU
2	B	319	LYS
2	B	328	LYS
2	B	361	LYS
2	B	364	ASN
2	B	376	GLN
2	B	392	LEU
2	B	394	LEU
2	B	430	THR
2	B	432	SER
2	B	433	ASP
2	B	438	VAL
2	B	447	ARG
2	B	491	VAL
2	B	497	LYS
2	B	501	ILE
2	B	504	THR
2	B	507	LYS
2	B	528	GLU
2	B	531	LYS
2	B	535	LYS
2	B	539	LYS
2	B	544	SER
2	B	545	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	46	ASN
1	A	77	HIS
1	A	87	HIS
1	A	153	GLN
1	A	244	HIS
1	A	281	ASN
1	A	300	GLN
1	A	383	HIS
1	A	415	HIS
1	A	461	ASN
1	A	519	GLN
1	A	572	ASN

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Mol	Chain	Res	Type
1	A	606	ASN
1	A	636	ASN
2	B	57	ASN
2	B	84	GLN
2	B	96	ASN
2	B	227	HIS
2	B	249	HIS
2	B	279	GLN
2	B	376	GLN
2	B	505	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	A	668	-	4,4,4	0.18	0	6,6,6	0.12	0
4	SO4	A	669	-	4,4,4	0.19	0	6,6,6	0.37	0
4	SO4	A	670	-	4,4,4	0.22	0	6,6,6	0.40	0
5	BEF	A	671	6	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ADP	A	672	3,5	25,29,29	1.03	1 (4%)	24,45,45	1.60	2 (8%)
4	SO4	B	559	-	4,4,4	0.12	0	6,6,6	0.28	0
6	ADP	B	560	-	25,29,29	1.11	2 (8%)	24,45,45	2.24	6 (25%)

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	SO4	A	668	-	-	0/0/0/0	0/0/0/0
4	SO4	A	669	-	-	0/0/0/0	0/0/0/0
4	SO4	A	670	-	-	0/0/0/0	0/0/0/0
5	BEF	A	671	6	-	0/0/0/0	0/0/0/0
6	ADP	A	672	3,5	-	0/12/32/32	0/3/3/3
4	SO4	B	559	-	-	0/0/0/0	0/0/0/0
6	ADP	B	560	-	-	0/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	560	ADP	PB-O3A	2.35	1.63	1.60
6	B	560	ADP	C5-C4	2.99	1.47	1.40
6	A	672	ADP	C5-C4	3.34	1.48	1.40

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	560	ADP	N3-C2-N1	-7.02	122.74	128.86
6	A	672	ADP	N3-C2-N1	-5.62	123.96	128.86
6	B	560	ADP	C4-C5-N7	-4.68	104.89	109.41
6	B	560	ADP	C4'-O4'-C1'	-2.66	106.94	109.77
6	A	672	ADP	C4-C5-N7	-2.59	106.91	109.41
6	B	560	ADP	C1'-N9-C4	-2.06	123.07	126.64
6	B	560	ADP	O3B-PB-O2B	2.30	116.90	107.61
6	B	560	ADP	C2-N1-C6	3.01	124.03	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	672	ADP	1	0
6	B	560	ADP	5	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	649/668 (97%)	-0.28	5 (0%)	86 72	10, 42, 114, 147	0
2	B	540/554 (97%)	-0.23	4 (0%)	87 76	22, 50, 99, 136	0
All	All	1189/1222 (97%)	-0.26	9 (0%)	86 72	10, 47, 107, 147	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	508	GLY	3.5
1	A	591	PRO	2.9
1	A	516	ASP	2.7
2	B	109	GLY	2.5
2	B	383	ASP	2.3
2	B	95	VAL	2.2
1	A	639	ARG	2.2
1	A	510	PRO	2.1
1	A	592	PHE	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(Å ²)	Q<0.9
4	SO4	A	669	5/5	0.91	0.33	12.00	76,79,80,82	0
3	MG	A	667	1/1	0.97	0.41	9.79	14,14,14,14	0
5	BEF	A	671	4/4	0.97	0.34	6.12	39,39,39,39	0
4	SO4	A	670	5/5	0.87	0.28	4.10	103,106,108,109	0
4	SO4	A	668	5/5	0.97	0.34	3.86	81,83,85,86	0
7	CL	B	556	1/1	0.86	0.22	1.36	65,65,65,65	0
6	ADP	B	560	27/27	0.93	0.23	1.31	60,60,60,60	0
6	ADP	A	672	27/27	0.96	0.23	1.13	44,44,44,44	0
4	SO4	B	559	5/5	0.96	0.24	0.95	70,72,74,75	0
7	CL	B	555	1/1	0.85	0.15	-1.68	69,69,69,69	0
7	CL	B	557	1/1	0.97	0.15	-	48,48,48,48	0
3	MG	B	558	1/1	0.94	0.34	-	27,27,27,27	0

6.5 Other polymers

There are no such residues in this entry.