Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2024 – 10:12 PM EST

PDB ID	:	1DK5
Title	:	CRYSTAL STRUCTURE OF ANNEXIN 24(CA32) FROM CAPSICUM ANNUUM
Authors	:	Hofmann, A.; Proust, J.; Dorowski, A.; Schantz, R.; Huber, R.
Deposited on	:	1999-12-06
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

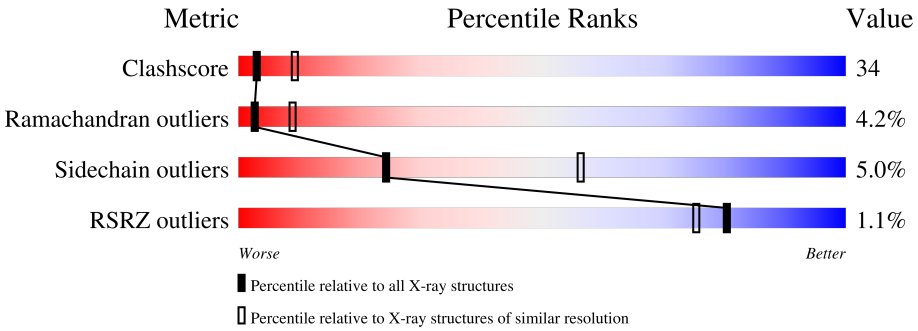
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 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	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	322	46% 47% 5%
1	B	322	45% 42% 9%

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
2	SO4	A	804	-	-	X	-
2	SO4	A	806	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	808	-	-	X	-
2	SO4	B	824	-	-	X	-
2	SO4	B	826	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5572 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.

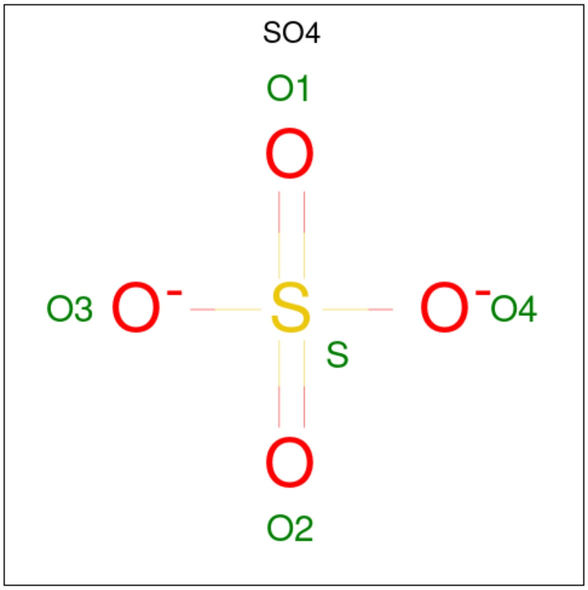
- Molecule 1 is a protein called ANNEXIN 24(CA32).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2550	1603	458	485	4			
1	B	314	Total	C	N	O	S	0	0	0
			2529	1590	450	485	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP Q42657
A	2	ALA	-	expression tag	UNP Q42657
A	3	HIS	-	expression tag	UNP Q42657
A	4	HIS	-	expression tag	UNP Q42657
A	5	HIS	-	expression tag	UNP Q42657
A	6	HIS	-	expression tag	UNP Q42657
A	7	HIS	-	expression tag	UNP Q42657
A	8	HIS	-	expression tag	UNP Q42657
B	401	MET	-	expression tag	UNP Q42657
B	402	ALA	-	expression tag	UNP Q42657
B	403	HIS	-	expression tag	UNP Q42657
B	404	HIS	-	expression tag	UNP Q42657
B	405	HIS	-	expression tag	UNP Q42657
B	406	HIS	-	expression tag	UNP Q42657
B	407	HIS	-	expression tag	UNP Q42657
B	408	HIS	-	expression tag	UNP Q42657

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 3 is water.

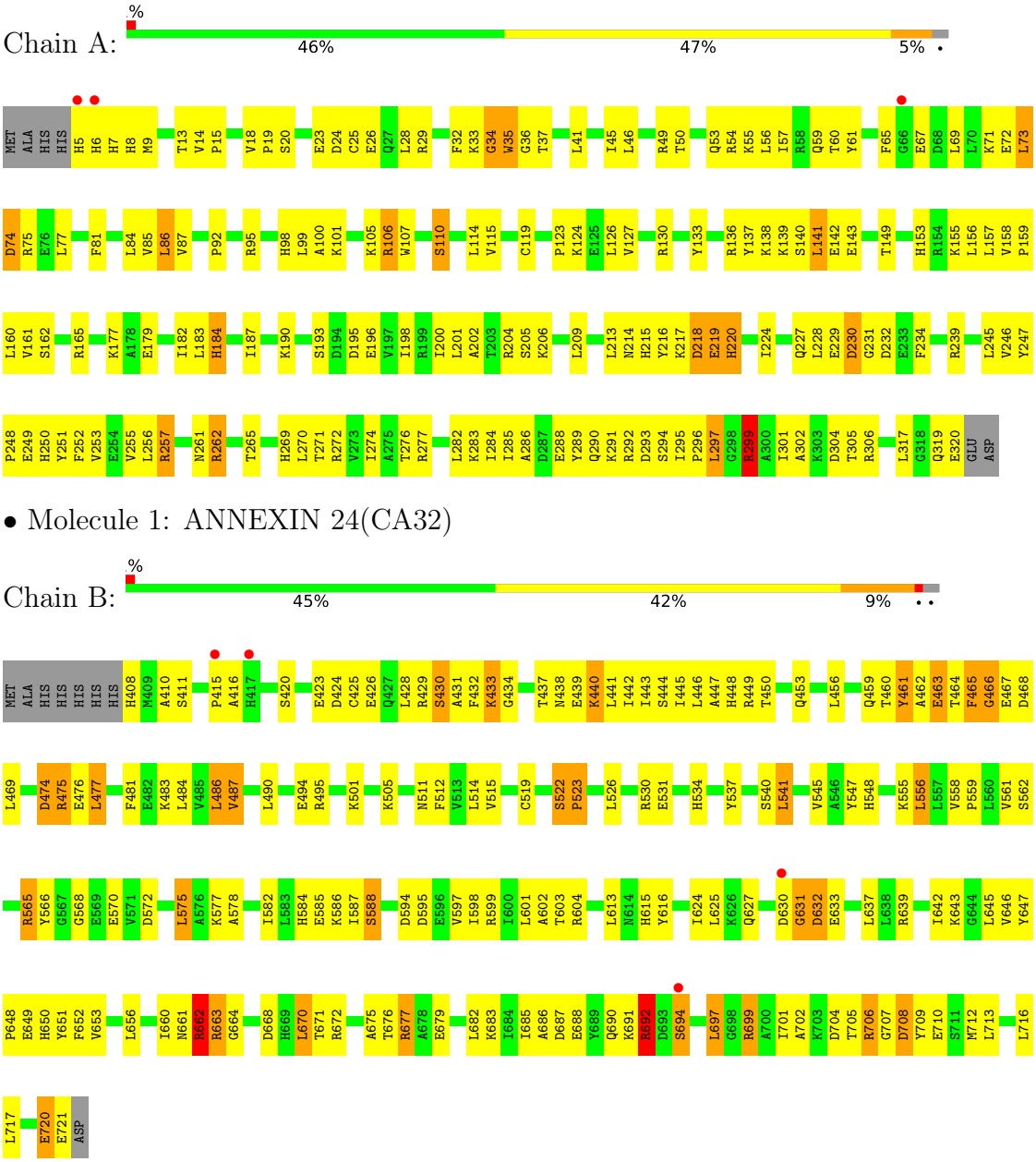
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	181	Total O 181 181	0	0
3	B	147	Total O 147 147	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: ANNEXIN 24(CA32)

Chain A:



• Molecule 1: ANNEXIN 24(CA32)

Chain B:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	96.76Å 96.76Å 173.39Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.80 24.81 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.7 (50.00-2.80) 98.4 (24.81-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.36 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.216 , 0.316 0.231 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	59.3	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 62.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5572	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.83	1/2596 (0.0%)	0.93	5/3506 (0.1%)
1	B	0.81	3/2572 (0.1%)	1.03	12/3473 (0.3%)
All	All	0.82	4/5168 (0.1%)	0.98	17/6979 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	110	SER	CB-OG	-21.51	1.14	1.42
1	B	631	GLY	CA-C	9.74	1.67	1.51
1	B	631	GLY	N-CA	6.54	1.55	1.46
1	B	664	GLY	CA-C	5.27	1.60	1.51

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	630	ASP	O-C-N	-7.80	109.94	123.20
1	B	662	ARG	NE-CZ-NH2	7.40	124.00	120.30
1	B	692	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	B	663	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	B	694	SER	N-CA-CB	7.19	121.29	110.50
1	A	297	LEU	CA-CB-CG	6.83	131.00	115.30
1	B	677	ARG	NE-CZ-NH2	6.72	123.66	120.30
1	A	34	GLY	N-CA-C	6.39	129.08	113.10
1	B	672	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	A	306	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	B	720	GLU	N-CA-C	-6.09	94.55	111.00
1	B	699	ARG	NE-CZ-NH2	5.91	123.25	120.30
1	B	630	ASP	CB-CA-C	-5.67	99.06	110.40
1	A	141	LEU	CA-CB-CG	5.41	127.75	115.30
1	A	114	LEU	CA-CB-CG	5.25	127.37	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	630	ASP	CA-C-N	5.09	126.38	116.20
1	B	468	ASP	N-CA-C	-5.08	97.27	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	2550	0	2551	195	0
1	B	2529	0	2536	160	0
2	A	70	0	0	15	0
2	B	95	0	0	9	0
3	A	181	0	0	16	0
3	B	147	0	0	5	0
All	All	5572	0	5087	355	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 34.

All (355) 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:179:GLU:HG2	1:A:200:ILE:HD13	1.15	1.12
1:B:662:ARG:HG3	1:B:663:ARG:H	1.01	1.12
1:B:706:ARG:HD3	1:B:707:GLY:H	1.22	1.04
1:A:239:ARG:HD3	3:A:977:HOH:O	1.58	1.02
1:B:599:ARG:HG2	2:B:826:SO4:O4	1.57	1.01
1:A:140:SER:HB2	1:A:143:GLU:HB2	1.41	0.99
1:A:55:LYS:O	1:A:59:GLN:HG3	1.62	0.98
1:A:179:GLU:HG2	1:A:200:ILE:CD1	1.94	0.97
1:A:69:LEU:O	1:A:73:LEU:HD23	1.68	0.94
1:B:662:ARG:CG	1:B:663:ARG:H	1.80	0.93
1:A:155:LYS:HG2	1:A:198:ILE:HD13	1.49	0.93
1:B:662:ARG:HG3	1:B:663:ARG:N	1.84	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ARG:HE	1:A:257:ARG:HA	1.37	0.90
1:A:20:SER:OG	1:A:23:GLU:HG3	1.70	0.90
1:A:183:LEU:O	1:A:187:ILE:HG12	1.76	0.86
1:A:296:PRO:HD2	1:A:299:ARG:HG3	1.57	0.85
1:A:7:HIS:CE1	1:A:8:HIS:HB3	2.12	0.84
1:B:475:ARG:HG3	1:B:475:ARG:HH11	1.42	0.84
1:B:441:LEU:O	1:B:445:ILE:HG13	1.77	0.83
1:A:190:LYS:HD2	3:A:1002:HOH:O	1.77	0.83
1:B:408:HIS:O	1:B:683:LYS:HD3	1.79	0.83
1:A:100:ALA:HB1	1:A:141:LEU:HD13	1.60	0.82
1:A:262:ARG:NE	1:A:262:ARG:H	1.78	0.81
1:B:706:ARG:HD3	1:B:707:GLY:N	1.96	0.80
1:B:430:SER:O	1:B:433:LYS:HD2	1.81	0.80
1:A:15:PRO:HD2	1:A:18:VAL:HG12	1.64	0.79
1:A:179:GLU:CG	1:A:200:ILE:HD13	2.08	0.79
1:A:5:HIS:N	1:A:50:THR:HG21	1.97	0.79
1:B:477:LEU:HD11	1:B:486:LEU:HD12	1.65	0.78
1:B:501:LYS:HD2	1:B:501:LYS:O	1.82	0.78
1:B:577:LYS:HG3	1:B:615:HIS:NE2	1.98	0.78
1:A:140:SER:HB2	1:A:143:GLU:CB	2.14	0.78
1:B:706:ARG:CD	1:B:707:GLY:H	1.96	0.78
1:A:230:ASP:CG	1:A:231:GLY:N	2.35	0.77
1:A:153:HIS:HD2	2:A:804:SO4:O1	1.66	0.77
1:B:431:ALA:HA	1:B:438:ASN:OD1	1.85	0.76
1:A:35:TRP:O	1:A:37:THR:N	2.18	0.75
1:A:319:GLN:O	1:A:320:GLU:HG3	1.86	0.75
1:B:701:ILE:O	1:B:705:THR:HB	1.86	0.74
1:A:257:ARG:HA	1:A:257:ARG:NE	2.01	0.74
1:A:9:MET:O	1:A:283:LYS:HB3	1.87	0.74
1:B:420:SER:OG	1:B:423:GLU:HG3	1.87	0.74
1:B:705:THR:HG22	1:B:710:GLU:HB2	1.71	0.73
1:A:155:LYS:HG2	1:A:198:ILE:CD1	2.17	0.73
1:B:613:LEU:HD22	1:B:624:ILE:HG21	1.70	0.73
1:B:565:ARG:NH2	1:B:601:LEU:O	2.22	0.73
1:B:495:ARG:HH11	1:B:676:THR:HA	1.53	0.72
1:A:214:ASN:O	1:A:217:LYS:HG2	1.89	0.72
1:A:249:GLU:N	1:A:249:GLU:OE2	2.23	0.72
1:A:249:GLU:HB2	2:A:806:SO4:S	2.29	0.72
1:B:639:ARG:O	1:B:643:LYS:HB2	1.90	0.72
1:A:165:ARG:NH2	1:A:201:LEU:O	2.23	0.71
1:A:130:ARG:HB3	2:A:808:SO4:O3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:LYS:HE3	3:A:1073:HOH:O	1.91	0.71
1:A:187:ILE:HD12	1:A:228:LEU:HD21	1.71	0.70
1:B:441:LEU:CD2	1:B:445:ILE:HD11	2.20	0.70
1:B:565:ARG:NH2	1:B:645:LEU:HD11	2.07	0.70
1:A:5:HIS:N	1:A:50:THR:CG2	2.54	0.70
1:A:130:ARG:NE	2:A:808:SO4:O1	2.25	0.70
1:A:95:ARG:O	1:A:99:LEU:HG	1.92	0.69
1:A:7:HIS:CG	1:A:8:HIS:H	2.10	0.69
1:A:261:ASN:ND2	1:A:262:ARG:HH21	1.90	0.69
1:A:7:HIS:CG	1:A:8:HIS:N	2.59	0.69
1:A:101:LYS:HE3	1:A:105:LYS:HE2	1.74	0.68
1:A:261:ASN:HD22	1:A:262:ARG:HH21	1.41	0.68
1:B:572:ASP:OD2	1:B:575:LEU:HB2	1.94	0.68
1:A:136:ARG:NE	3:A:913:HOH:O	2.25	0.68
1:B:541:LEU:O	1:B:545:VAL:HG23	1.94	0.67
1:B:415:PRO:HD3	1:B:448:HIS:HB3	1.74	0.67
1:B:440:LYS:HD2	1:B:440:LYS:O	1.94	0.67
1:A:69:LEU:O	1:A:72:GLU:HB3	1.94	0.67
1:B:512:PHE:O	1:B:515:VAL:HG22	1.95	0.67
1:A:232:ASP:HB2	2:A:805:SO4:O1	1.94	0.67
1:B:475:ARG:HG3	1:B:475:ARG:NH1	2.05	0.67
1:B:671:THR:OG1	3:B:949:HOH:O	2.13	0.66
1:A:149:THR:HA	2:A:804:SO4:O4	1.96	0.66
1:B:484:LEU:HD13	1:B:671:THR:HG23	1.77	0.66
1:B:511:ASN:HA	1:B:514:LEU:HD12	1.76	0.66
1:A:262:ARG:H	1:A:262:ARG:HE	1.42	0.66
1:A:317:LEU:O	1:A:317:LEU:HG	1.94	0.66
1:A:69:LEU:HD12	1:A:73:LEU:HD22	1.77	0.66
1:A:261:ASN:ND2	1:A:262:ARG:NH2	2.44	0.66
1:A:142:GLU:OE1	2:A:808:SO4:S	2.54	0.65
1:A:140:SER:HB2	1:A:143:GLU:H	1.62	0.65
1:A:69:LEU:HD12	1:A:73:LEU:CD2	2.26	0.65
1:A:136:ARG:HG3	1:A:137:TYR:CE2	2.30	0.65
1:B:469:LEU:HD23	1:B:469:LEU:O	1.97	0.65
1:B:481:PHE:HD2	3:B:1035:HOH:O	1.79	0.64
1:B:459:GLN:O	1:B:463:GLU:HG2	1.97	0.64
1:B:476:GLU:OE2	2:B:833:SO4:O1	2.16	0.64
1:B:650:HIS:NE2	1:B:688:GLU:OE1	2.31	0.64
1:A:28:LEU:HD21	1:A:46:LEU:HD21	1.77	0.64
1:B:477:LEU:CD1	1:B:486:LEU:HD12	2.28	0.64
1:A:37:THR:O	1:A:37:THR:HG22	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:GLU:O	3:A:1150:HOH:O	2.16	0.63
1:A:182:ILE:HG21	1:A:196:GLU:HB3	1.80	0.63
1:B:428:LEU:O	1:B:431:ALA:HB3	1.99	0.63
1:B:649:GLU:O	1:B:653:VAL:HG23	1.99	0.62
1:A:213:LEU:HD13	1:A:224:ILE:HG21	1.81	0.62
1:B:501:LYS:HG2	1:B:537:TYR:CE2	2.34	0.62
1:A:41:LEU:O	1:A:45:ILE:HG13	1.98	0.62
1:B:683:LYS:NZ	3:B:1074:HOH:O	2.32	0.62
1:A:50:THR:H	1:A:53:GLN:NE2	1.99	0.61
1:A:230:ASP:OD2	1:A:231:GLY:N	2.34	0.61
1:B:577:LYS:HG3	1:B:615:HIS:CE1	2.35	0.61
1:A:297:LEU:HD13	1:A:301:ILE:HD12	1.82	0.61
1:A:6:HIS:CD2	1:A:14:VAL:HG22	2.36	0.61
1:B:710:GLU:HG2	1:B:710:GLU:O	2.00	0.60
1:A:20:SER:N	1:A:23:GLU:OE1	2.30	0.60
1:A:217:LYS:HE2	3:A:1083:HOH:O	2.01	0.60
1:B:646:VAL:O	1:B:648:PRO:HD2	2.01	0.60
1:B:428:LEU:HD13	1:B:445:ILE:HD12	1.84	0.60
1:A:53:GLN:O	1:A:57:ILE:HG13	2.02	0.60
1:A:98:HIS:ND1	2:A:802:SO4:O4	2.33	0.60
1:B:656:LEU:HD13	1:B:697:LEU:HD11	1.83	0.59
1:A:56:LEU:O	1:A:60:THR:HG23	2.01	0.59
1:B:410:ALA:O	1:B:683:LYS:HB2	2.02	0.59
1:B:495:ARG:NH1	1:B:676:THR:HA	2.17	0.59
1:B:511:ASN:O	1:B:515:VAL:HG13	2.02	0.59
1:A:209:LEU:HD21	1:A:245:LEU:HD13	1.84	0.59
1:B:432:PHE:O	1:B:434:GLY:N	2.36	0.59
1:B:720:GLU:C	1:B:721:GLU:OE1	2.42	0.59
1:A:253:VAL:HG21	1:A:288:GLU:HB2	1.85	0.58
1:B:639:ARG:NE	2:B:832:SO4:O2	2.36	0.58
1:A:45:ILE:O	1:A:49:ARG:HG2	2.03	0.58
1:A:9:MET:HG2	1:A:284:ILE:HD11	1.85	0.58
1:A:155:LYS:NZ	1:A:195:ASP:OD1	2.29	0.58
1:A:7:HIS:CE1	1:A:9:MET:HG3	2.38	0.58
1:B:526:LEU:O	1:B:530:ARG:HG3	2.04	0.58
1:A:209:LEU:CD2	1:A:245:LEU:HD13	2.34	0.57
1:B:460:THR:HA	1:B:463:GLU:HG2	1.86	0.57
1:A:206:LYS:HG3	3:A:1030:HOH:O	2.05	0.57
1:B:613:LEU:HD22	1:B:624:ILE:CG2	2.33	0.57
1:A:270:LEU:O	1:A:274:ILE:HG12	2.04	0.57
1:A:124:LYS:HA	1:A:127:VAL:HG12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:GLU:O	1:A:253:VAL:HG23	2.04	0.56
1:B:462:ALA:O	1:B:464:THR:N	2.38	0.56
1:B:699:ARG:O	1:B:702:ALA:N	2.37	0.56
1:A:165:ARG:NH2	1:A:202:ALA:HA	2.19	0.56
1:B:438:ASN:O	1:B:439:GLU:C	2.43	0.56
1:A:71:LYS:HE2	3:A:1166:HOH:O	2.06	0.56
1:B:461:TYR:O	1:B:461:TYR:CD1	2.58	0.56
1:A:140:SER:CB	1:A:143:GLU:H	2.19	0.56
1:A:196:GLU:O	1:A:200:ILE:HG13	2.06	0.56
1:B:613:LEU:CD2	1:B:624:ILE:HG21	2.35	0.56
1:A:299:ARG:O	1:A:302:ALA:N	2.39	0.55
1:B:450:THR:OG1	1:B:453:GLN:HG3	2.06	0.55
1:A:87:VAL:O	1:A:95:ARG:HD3	2.07	0.54
1:A:123:PRO:HD2	2:A:813:SO4:O4	2.07	0.54
1:A:317:LEU:O	1:A:317:LEU:CG	2.55	0.54
1:A:138:LYS:O	1:A:139:LYS:HG3	2.06	0.54
1:B:483:LYS:O	1:B:487:VAL:HG22	2.07	0.54
1:A:71:LYS:HA	1:A:74:ASP:OD1	2.08	0.54
1:B:429:ARG:C	1:B:431:ALA:H	2.11	0.54
1:A:50:THR:O	1:A:54:ARG:HG3	2.07	0.54
1:A:69:LEU:CD1	1:A:73:LEU:HD22	2.38	0.54
1:B:566:TYR:CE1	1:B:568:GLY:N	2.76	0.54
1:A:74:ASP:HA	1:A:86:LEU:HD21	1.90	0.53
1:A:119:CYS:HB3	1:A:245:LEU:HG	1.90	0.53
1:A:205:SER:O	1:A:209:LEU:HB2	2.07	0.53
1:A:256:LEU:HD13	1:A:297:LEU:HD21	1.91	0.53
1:A:299:ARG:HD2	3:A:907:HOH:O	2.08	0.53
1:A:304:ASP:O	1:A:305:THR:HG22	2.08	0.53
1:A:126:LEU:O	1:A:126:LEU:HG	2.07	0.53
1:B:558:VAL:O	1:B:562:SER:HB2	2.09	0.53
1:A:87:VAL:HG13	1:A:95:ARG:HG3	1.91	0.53
1:B:613:LEU:HD11	1:B:642:ILE:CG2	2.39	0.53
1:B:687:ASP:O	1:B:690:GLN:HG2	2.09	0.53
1:A:213:LEU:HD13	1:A:224:ILE:CG2	2.39	0.53
1:A:230:ASP:CG	1:A:231:GLY:H	2.12	0.52
1:B:411:SER:HB2	1:B:717:LEU:O	2.10	0.52
1:B:437:THR:C	1:B:438:ASN:HD22	2.11	0.52
1:A:261:ASN:HB3	1:A:262:ARG:NH2	2.23	0.52
1:B:540:SER:O	1:B:541:LEU:C	2.47	0.52
1:A:124:LYS:O	1:A:127:VAL:CG1	2.57	0.52
1:A:130:ARG:HH12	1:A:162:SER:C	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:LYS:HE3	1:A:198:ILE:HD12	1.92	0.52
1:A:269:HIS:CD2	1:A:272:ARG:HH12	2.28	0.52
1:A:153:HIS:CD2	2:A:804:SO4:O1	2.56	0.52
1:B:648:PRO:O	1:B:651:TYR:HB3	2.09	0.52
1:A:283:LYS:HG3	3:A:856:HOH:O	2.10	0.51
1:A:250:HIS:CE1	3:A:992:HOH:O	2.63	0.51
1:B:438:ASN:O	1:B:441:LEU:N	2.39	0.51
1:A:246:VAL:HG12	1:A:247:TYR:CE1	2.46	0.51
1:B:462:ALA:C	1:B:464:THR:N	2.60	0.51
1:B:519:CYS:SG	1:B:645:LEU:HG	2.50	0.51
1:B:441:LEU:HD22	1:B:445:ILE:HD11	1.93	0.51
1:B:585:GLU:HG3	1:B:586:LYS:N	2.26	0.51
1:B:441:LEU:HD23	1:B:445:ILE:HD11	1.92	0.51
1:B:442:ILE:HG22	1:B:446:LEU:HD12	1.93	0.51
1:A:216:TYR:CE1	1:A:224:ILE:HD13	2.46	0.50
1:A:304:ASP:O	1:A:305:THR:CG2	2.59	0.50
1:B:587:ILE:HG21	1:B:627:GLN:CG	2.41	0.50
1:A:290:GLN:O	1:A:291:LYS:C	2.49	0.50
1:B:632:ASP:OD2	1:B:633:GLU:N	2.44	0.50
1:B:682:LEU:HA	1:B:685:ILE:HD12	1.93	0.50
1:A:136:ARG:HG3	1:A:137:TYR:CD2	2.47	0.50
1:B:660:ILE:HD12	1:B:660:ILE:N	2.26	0.50
1:A:130:ARG:NH1	1:A:162:SER:HA	2.26	0.50
1:A:6:HIS:CD2	1:A:14:VAL:H	2.30	0.50
1:A:124:LYS:O	1:A:127:VAL:HG12	2.12	0.50
1:B:474:ASP:O	1:B:475:ARG:C	2.51	0.49
1:B:578:ALA:O	1:B:582:ILE:HG13	2.12	0.49
1:B:570:GLU:CD	1:B:570:GLU:H	2.16	0.49
1:A:24:ASP:O	1:A:28:LEU:HB2	2.13	0.49
1:A:67:GLU:OE2	1:A:72:GLU:OE2	2.30	0.49
1:B:456:LEU:O	1:B:460:THR:HG23	2.12	0.49
1:B:683:LYS:O	1:B:686:ALA:HB3	2.12	0.49
1:B:494:GLU:HB3	2:B:824:SO4:O4	2.12	0.49
1:B:705:THR:HG21	1:B:713:LEU:HD12	1.94	0.49
1:A:142:GLU:OE1	2:A:808:SO4:O1	2.29	0.49
1:B:490:LEU:HD22	2:B:824:SO4:O4	2.13	0.49
1:A:5:HIS:CD2	3:A:998:HOH:O	2.64	0.49
1:A:133:TYR:HD1	1:A:139:LYS:O	1.96	0.49
1:A:7:HIS:CD2	1:A:8:HIS:H	2.30	0.49
1:A:84:LEU:HD13	1:A:271:THR:HG23	1.94	0.49
1:B:501:LYS:HD2	1:B:501:LYS:C	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ASP:C	1:A:305:THR:CG2	2.81	0.49
1:A:248:PRO:HG2	1:A:249:GLU:OE2	2.13	0.49
1:A:251:TYR:O	1:A:255:VAL:HG23	2.13	0.49
1:A:124:LYS:HA	1:A:127:VAL:CG1	2.43	0.48
1:B:465:PHE:CD1	1:B:465:PHE:N	2.80	0.48
1:A:7:HIS:HE1	1:A:9:MET:HG3	1.76	0.48
1:A:293:ASP:HB3	1:A:295:ILE:HG13	1.95	0.48
1:A:282:LEU:HD12	1:A:285:ILE:HB	1.95	0.48
1:A:75:ARG:HE	1:A:75:ARG:HB2	1.44	0.48
1:A:256:LEU:HD23	1:A:256:LEU:HA	1.63	0.48
1:A:158:VAL:N	1:A:159:PRO:HD2	2.29	0.48
1:B:459:GLN:O	1:B:462:ALA:HB3	2.13	0.48
1:B:660:ILE:HD11	1:B:670:LEU:HG	1.95	0.48
1:A:156:LEU:HD13	1:A:160:LEU:HD12	1.96	0.48
1:A:74:ASP:O	1:A:74:ASP:CG	2.52	0.48
1:A:26:GLU:N	3:A:857:HOH:O	2.47	0.48
1:B:461:TYR:O	1:B:461:TYR:HD1	1.96	0.48
1:A:157:LEU:O	1:A:161:VAL:HG13	2.14	0.47
1:A:304:ASP:C	1:A:305:THR:HG23	2.34	0.47
1:B:425:CYS:SG	1:B:461:TYR:HB2	2.54	0.47
1:A:126:LEU:HD21	1:A:161:VAL:O	2.14	0.47
1:B:460:THR:HA	1:B:463:GLU:CG	2.44	0.47
1:A:214:ASN:HA	1:A:217:LYS:CD	2.45	0.47
1:A:61:TYR:CD1	1:A:61:TYR:O	2.67	0.47
1:B:505:LYS:HE2	1:B:505:LYS:HB3	1.62	0.47
1:A:5:HIS:HD2	3:A:998:HOH:O	1.98	0.47
1:B:431:ALA:O	1:B:437:THR:HG23	2.15	0.47
1:B:565:ARG:NH2	1:B:645:LEU:CD1	2.78	0.47
1:A:86:LEU:O	1:A:87:VAL:C	2.52	0.47
1:B:441:LEU:O	1:B:445:ILE:CG1	2.57	0.47
1:B:461:TYR:CD1	1:B:461:TYR:C	2.89	0.47
1:A:81:PHE:O	1:A:85:VAL:HG23	2.15	0.46
1:A:249:GLU:HB2	2:A:806:SO4:O1	2.15	0.46
1:A:41:LEU:O	1:A:41:LEU:HD23	2.15	0.46
1:A:290:GLN:O	1:A:294:SER:N	2.38	0.46
1:B:425:CYS:O	1:B:426:GLU:C	2.54	0.46
1:B:594:ASP:O	1:B:597:VAL:N	2.47	0.46
1:A:49:ARG:HA	1:A:53:GLN:NE2	2.31	0.46
1:B:662:ARG:CG	1:B:663:ARG:N	2.52	0.46
1:A:156:LEU:HD22	1:A:156:LEU:O	2.16	0.46
1:B:484:LEU:HD22	1:B:713:LEU:CD2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:599:ARG:NE	2:B:826:SO4:O3	2.48	0.46
1:B:708:ASP:OD1	1:B:708:ASP:N	2.49	0.46
1:A:18:VAL:HA	1:A:19:PRO:HD3	1.80	0.45
1:A:32:PHE:CE2	1:A:72:GLU:HG2	2.52	0.45
1:A:256:LEU:HD13	1:A:297:LEU:CD2	2.46	0.45
1:B:495:ARG:NH1	1:B:675:ALA:O	2.48	0.45
1:B:697:LEU:HD22	1:B:701:ILE:HG13	1.98	0.45
1:B:437:THR:C	1:B:438:ASN:ND2	2.69	0.45
1:B:512:PHE:CE1	1:B:637:LEU:HD23	2.51	0.45
1:B:587:ILE:HG21	1:B:627:GLN:HG3	1.99	0.45
1:B:709:TYR:O	1:B:713:LEU:HG	2.16	0.45
1:B:445:ILE:O	1:B:449:ARG:HG2	2.16	0.45
1:A:297:LEU:HD13	1:A:301:ILE:CD1	2.45	0.45
1:B:462:ALA:O	1:B:463:GLU:C	2.55	0.45
1:A:142:GLU:OE2	2:A:808:SO4:O2	2.34	0.45
1:A:286:ALA:O	1:A:289:TYR:HB3	2.16	0.45
1:A:29:ARG:HG2	1:A:65:PHE:CZ	2.52	0.45
1:B:428:LEU:HD23	1:B:469:LEU:HD11	1.99	0.45
1:B:555:LYS:HG2	1:B:598:ILE:CD1	2.47	0.45
1:A:261:ASN:CB	1:A:262:ARG:NH2	2.79	0.45
1:B:587:ILE:HG22	1:B:588:SER:N	2.32	0.45
1:A:115:VAL:HG13	1:A:119:CYS:SG	2.57	0.44
1:A:218:ASP:O	1:A:219:GLU:C	2.56	0.44
1:B:429:ARG:NH1	1:B:465:PHE:CG	2.86	0.44
1:B:474:ASP:O	1:B:476:GLU:N	2.49	0.44
1:A:69:LEU:CD1	1:A:73:LEU:CD2	2.94	0.44
1:A:155:LYS:HE3	1:A:193:SER:O	2.17	0.44
1:B:661:ASN:O	1:B:704:ASP:OD1	2.36	0.44
1:A:218:ASP:HB2	1:A:219:GLU:H	1.51	0.44
1:B:447:ALA:HB2	1:B:712:MET:CE	2.48	0.43
1:B:420:SER:OG	1:B:423:GLU:CG	2.62	0.43
1:A:119:CYS:O	1:A:206:LYS:HE2	2.19	0.43
1:A:140:SER:HB3	1:A:142:GLU:OE1	2.17	0.43
1:B:603:THR:OG1	2:B:826:SO4:O4	2.36	0.43
1:A:142:GLU:HB2	1:A:158:VAL:HG13	2.00	0.43
1:A:257:ARG:NH2	1:A:289:TYR:OH	2.51	0.43
1:A:182:ILE:CG2	1:A:196:GLU:HB3	2.48	0.43
1:A:289:TYR:O	1:A:292:ARG:HB3	2.19	0.43
1:B:428:LEU:CD1	1:B:445:ILE:HD12	2.48	0.43
1:B:429:ARG:O	1:B:431:ALA:N	2.44	0.43
1:B:555:LYS:HG2	1:B:598:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:THR:HG21	1:B:465:PHE:CZ	2.53	0.43
1:A:49:ARG:HG2	1:A:49:ARG:HH11	1.84	0.43
1:B:424:ASP:O	1:B:428:LEU:HB2	2.19	0.43
1:B:461:TYR:O	1:B:465:PHE:HD1	2.02	0.43
1:B:625:LEU:HD23	1:B:625:LEU:HA	1.71	0.43
1:A:106:ARG:HG2	1:A:107:TRP:NE1	2.34	0.42
1:B:531:GLU:O	1:B:534:HIS:HB2	2.19	0.42
1:B:716:LEU:HD23	1:B:716:LEU:HA	1.82	0.42
1:A:35:TRP:C	1:A:37:THR:H	2.15	0.42
1:A:130:ARG:CZ	2:A:808:SO4:O1	2.68	0.42
1:B:575:LEU:HD11	1:B:604:ARG:CZ	2.49	0.42
1:B:652:PHE:CE2	1:B:677:ARG:CZ	3.02	0.42
1:A:33:LYS:NZ	3:A:921:HOH:O	2.46	0.42
1:A:156:LEU:HB2	1:A:234:PHE:HE1	1.85	0.42
1:A:216:TYR:OH	1:A:227:GLN:OE1	2.38	0.42
1:A:142:GLU:OE1	1:A:142:GLU:N	2.44	0.42
1:B:466:GLY:O	2:B:823:SO4:O1	2.38	0.42
1:A:60:THR:HG22	3:A:920:HOH:O	2.18	0.42
1:B:556:LEU:O	1:B:559:PRO:HG2	2.20	0.42
1:A:289:TYR:CE2	1:A:297:LEU:HA	2.55	0.41
1:B:475:ARG:NH1	1:B:475:ARG:CG	2.78	0.41
1:B:697:LEU:O	1:B:701:ILE:HG13	2.20	0.41
1:B:541:LEU:HD13	1:B:561:VAL:HB	2.02	0.41
1:A:140:SER:CB	1:A:143:GLU:HB2	2.30	0.41
1:A:276:THR:O	1:A:277:ARG:HD2	2.20	0.41
1:B:522:SER:O	1:B:523:PRO:C	2.59	0.41
1:A:293:ASP:O	1:A:294:SER:HB2	2.20	0.41
1:B:432:PHE:C	1:B:434:GLY:H	2.24	0.41
1:A:218:ASP:O	1:A:219:GLU:O	2.38	0.41
1:B:456:LEU:HD21	3:B:1104:HOH:O	2.19	0.41
1:B:565:ARG:NH2	1:B:602:ALA:HA	2.35	0.41
1:A:25:CYS:O	1:A:26:GLU:C	2.57	0.41
1:B:599:ARG:HG2	2:B:826:SO4:S	2.56	0.41
1:B:679:GLU:HG3	3:B:938:HOH:O	2.21	0.41
1:B:547:TYR:HD2	1:B:548:HIS:CE1	2.38	0.41
1:B:646:VAL:HG12	1:B:647:TYR:CD1	2.55	0.41
1:B:697:LEU:HD22	1:B:701:ILE:HD11	2.03	0.41
1:A:130:ARG:NH1	1:A:162:SER:C	2.74	0.41
1:A:184:HIS:CD2	1:A:220:HIS:ND1	2.89	0.41
1:A:209:LEU:HD12	1:A:209:LEU:HA	1.87	0.41
1:B:484:LEU:CD1	1:B:671:THR:HG23	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:660:ILE:N	1:B:660:ILE:CD1	2.84	0.41
1:A:130:ARG:NE	2:A:808:SO4:S	2.90	0.40
1:B:420:SER:HG	1:B:423:GLU:HG3	1.83	0.40
1:B:691:LYS:O	1:B:692:ARG:C	2.59	0.40
1:A:7:HIS:ND1	1:A:8:HIS:N	2.68	0.40
1:B:584:HIS:HB2	1:B:616:TYR:CE1	2.56	0.40
1:A:92:PRO:HG3	1:A:95:ARG:NH1	2.36	0.40
1:A:179:GLU:OE2	1:A:204:ARG:NH2	2.39	0.40
1:A:215:HIS:HA	1:A:218:ASP:OD2	2.20	0.40
1:B:425:CYS:O	1:B:428:LEU:N	2.54	0.40
1:A:74:ASP:HB2	1:A:77:LEU:HD21	2.04	0.40
1:A:183:LEU:HD23	1:A:183:LEU:HA	1.88	0.40
1:A:248:PRO:O	1:A:252:PHE:HD2	2.05	0.40
1:B:595:ASP:O	1:B:599:ARG:HB2	2.22	0.40
1:B:720:GLU:HG2	1:B:721:GLU:H	1.87	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	314/322 (98%)	276 (88%)	27 (9%)	11 (4%)	3 12
1	B	312/322 (97%)	253 (81%)	44 (14%)	15 (5%)	2 7
All	All	626/644 (97%)	529 (84%)	71 (11%)	26 (4%)	3 9

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	34	GLY
1	A	36	GLY
1	A	219	GLU

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Mol	Chain	Res	Type
1	B	416	ALA
1	B	433	LYS
1	B	467	GLU
1	B	662	ARG
1	A	229	GLU
1	A	230	ASP
1	B	430	SER
1	B	444	SER
1	B	466	GLY
1	B	631	GLY
1	B	632	ASP
1	A	218	ASP
1	B	463	GLU
1	B	475	ARG
1	A	184	HIS
1	A	220	HIS
1	A	299	ARG
1	B	565	ARG
1	A	86	LEU
1	A	106	ARG
1	B	692	ARG
1	B	694	SER
1	B	443	ILE

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	271/276 (98%)	262 (97%)	9 (3%)	38	72
1	B	269/276 (98%)	251 (93%)	18 (7%)	16	43
All	All	540/552 (98%)	513 (95%)	27 (5%)	24	56

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	THR
1	A	35	TRP
1	A	73	LEU
1	A	74	ASP
1	A	110	SER
1	A	257	ARG
1	A	262	ARG
1	A	265	THR
1	A	299	ARG
1	B	440	LYS
1	B	461	TYR
1	B	465	PHE
1	B	474	ASP
1	B	477	LEU
1	B	486	LEU
1	B	487	VAL
1	B	522	SER
1	B	523	PRO
1	B	541	LEU
1	B	556	LEU
1	B	575	LEU
1	B	588	SER
1	B	668	ASP
1	B	670	LEU
1	B	697	LEU
1	B	706	ARG
1	B	708	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	GLN
1	A	111	ASN
1	A	153	HIS
1	A	214	ASN
1	A	215	HIS
1	A	261	ASN
1	B	427	GLN
1	B	453	GLN
1	B	548	HIS
1	B	614	ASN
1	B	690	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

33 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	SO4	A	810	-	4,4,4	0.58	0	6,6,6	0.25	0
2	SO4	B	831	-	4,4,4	0.67	0	6,6,6	0.19	0
2	SO4	A	813	-	4,4,4	0.37	0	6,6,6	0.30	0
2	SO4	B	824	-	4,4,4	0.56	0	6,6,6	0.37	0
2	SO4	A	801	-	4,4,4	0.52	0	6,6,6	0.40	0
2	SO4	B	821	-	4,4,4	0.66	0	6,6,6	0.17	0
2	SO4	A	802	-	4,4,4	0.41	0	6,6,6	0.42	0
2	SO4	A	814	-	4,4,4	0.66	0	6,6,6	0.21	0
2	SO4	B	832	-	4,4,4	0.61	0	6,6,6	0.20	0
2	SO4	B	822	-	4,4,4	0.77	0	6,6,6	0.26	0
2	SO4	B	830	-	4,4,4	0.57	0	6,6,6	0.10	0
2	SO4	B	817	-	4,4,4	0.45	0	6,6,6	0.27	0
2	SO4	B	828	-	4,4,4	0.38	0	6,6,6	0.41	0
2	SO4	A	812	-	4,4,4	0.68	0	6,6,6	0.25	0
2	SO4	A	806	-	4,4,4	0.53	0	6,6,6	0.26	0
2	SO4	B	819	-	4,4,4	0.68	0	6,6,6	0.17	0
2	SO4	A	807	-	4,4,4	0.61	0	6,6,6	0.16	0
2	SO4	B	826	-	4,4,4	0.45	0	6,6,6	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	A	805	-	4,4,4	0.33	0	6,6,6	0.40	0
2	SO4	B	827	-	4,4,4	0.50	0	6,6,6	0.22	0
2	SO4	A	803	-	4,4,4	0.26	0	6,6,6	0.26	0
2	SO4	B	825	-	4,4,4	0.56	0	6,6,6	0.37	0
2	SO4	B	833	-	4,4,4	1.31	0	6,6,6	1.07	0
2	SO4	A	808	-	4,4,4	0.43	0	6,6,6	0.33	0
2	SO4	B	823	-	4,4,4	0.68	0	6,6,6	0.33	0
2	SO4	A	809	-	4,4,4	0.65	0	6,6,6	0.28	0
2	SO4	B	815	-	4,4,4	0.18	0	6,6,6	0.51	0
2	SO4	B	818	-	4,4,4	0.78	0	6,6,6	0.22	0
2	SO4	B	816	-	4,4,4	0.84	0	6,6,6	0.26	0
2	SO4	A	804	-	4,4,4	0.15	0	6,6,6	0.28	0
2	SO4	B	829	-	4,4,4	0.61	0	6,6,6	0.28	0
2	SO4	B	820	-	4,4,4	0.58	0	6,6,6	0.09	0
2	SO4	A	811	-	4,4,4	0.59	0	6,6,6	0.32	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	813	SO4	1	0
2	B	824	SO4	2	0
2	A	802	SO4	1	0
2	B	832	SO4	1	0
2	A	806	SO4	2	0
2	B	826	SO4	4	0
2	A	805	SO4	1	0
2	B	833	SO4	1	0
2	A	808	SO4	7	0
2	B	823	SO4	1	0
2	A	804	SO4	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	316/322 (98%)	-0.38	3 (0%)	84	80	24, 50, 72, 73	0
1	B	314/322 (97%)	-0.29	4 (1%)	77	72	25, 50, 72, 73	0
All	All	630/644 (97%)	-0.34	7 (1%)	80	75	24, 50, 72, 73	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	5	HIS	5.2
1	A	6	HIS	4.9
1	A	66	GLY	2.8
1	B	417	HIS	2.7
1	B	694	SER	2.4
1	B	630	ASP	2.3
1	B	415	PRO	2.2

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	833	5/5	0.81	0.44	64,64,64,64	0
2	SO4	B	822	5/5	0.85	0.23	69,72,72,72	0
2	SO4	A	809	5/5	0.85	0.32	68,71,72,72	0
2	SO4	B	821	5/5	0.86	0.32	71,72,72,72	0
2	SO4	B	818	5/5	0.89	0.45	72,72,72,72	0
2	SO4	B	819	5/5	0.90	0.37	68,69,72,72	0
2	SO4	B	816	5/5	0.91	0.52	72,72,72,72	0
2	SO4	A	811	5/5	0.91	0.34	72,72,72,72	0
2	SO4	A	814	5/5	0.91	0.45	70,72,72,72	0
2	SO4	B	823	5/5	0.92	0.48	72,72,72,72	0
2	SO4	B	827	5/5	0.92	0.24	66,67,70,72	0
2	SO4	A	807	5/5	0.92	0.52	72,72,72,72	0
2	SO4	A	806	5/5	0.93	0.21	69,69,72,72	0
2	SO4	B	824	5/5	0.93	0.29	71,72,72,72	0
2	SO4	B	826	5/5	0.93	0.53	72,72,72,72	0
2	SO4	A	808	5/5	0.93	0.28	72,72,72,72	0
2	SO4	A	812	5/5	0.93	0.33	72,72,72,72	0
2	SO4	A	801	5/5	0.94	0.25	69,70,72,72	0
2	SO4	A	805	5/5	0.94	0.12	64,67,67,71	0
2	SO4	B	828	5/5	0.94	0.17	63,64,68,70	0
2	SO4	B	825	5/5	0.94	0.23	69,72,72,72	0
2	SO4	B	830	5/5	0.95	0.28	72,72,72,72	0
2	SO4	B	831	5/5	0.95	0.47	72,72,72,72	0
2	SO4	B	832	5/5	0.95	0.24	72,72,72,72	0
2	SO4	B	829	5/5	0.95	0.24	69,71,72,72	0
2	SO4	B	817	5/5	0.96	0.09	56,68,70,72	0
2	SO4	A	802	5/5	0.96	0.11	56,63,68,68	0
2	SO4	A	810	5/5	0.96	0.42	71,72,72,72	0
2	SO4	A	803	5/5	0.96	0.14	56,58,61,64	0
2	SO4	B	820	5/5	0.97	0.34	68,72,72,72	0
2	SO4	A	813	5/5	0.98	0.16	64,69,71,71	0
2	SO4	A	804	5/5	0.99	0.10	42,44,49,52	0
2	SO4	B	815	5/5	0.99	0.09	41,42,46,47	0

6.5 Other polymers (i)

There are no such residues in this entry.