Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:11 PM GMT

PDB ID   :   1J7N
Title   :   Anthrax Toxin Lethal factor
Authors   :   Pannifer, A.D.; Wong, T.Y.; Schwarzenbacher, R.; Renatus, M.; Petosa, C.; Collier, R.J.; Bienkowska, J.; Lacy, D.B.; Park, S.; Leppla, S.H.; Hanna, P.; Liddington, R.C.
Deposited on   :   2001-05-17
Resolution   :   2.30 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.30 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	Percentile Ranks	Value
Clashscore		19
Ramachandran outliers		1.7%
Sidechain outliers		5.6%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
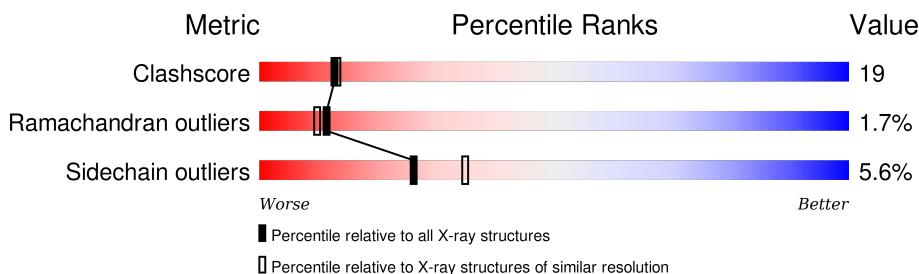
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

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 <=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.

Note EDS was not executed.

| Mol	Chain	Length	Quality of chain
1	A	776	59% 31% • 7%
1	B	776	64% 27% • 5%
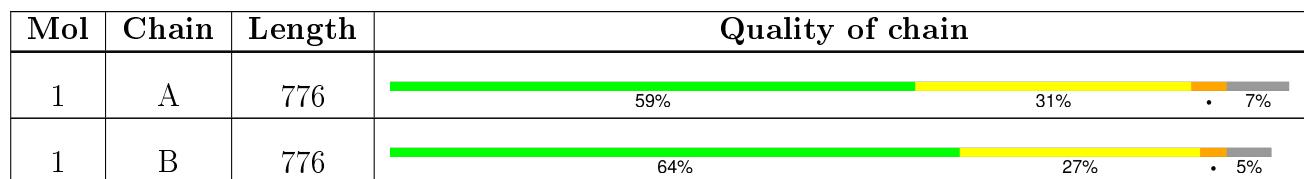
2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12924 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 Lethal Factor precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	725	Total 5947	C 3785	N 1003	O 1152	S 7	0	0	0
1	B	736	Total 6031	C 3832	N 1017	O 1175	S 7	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
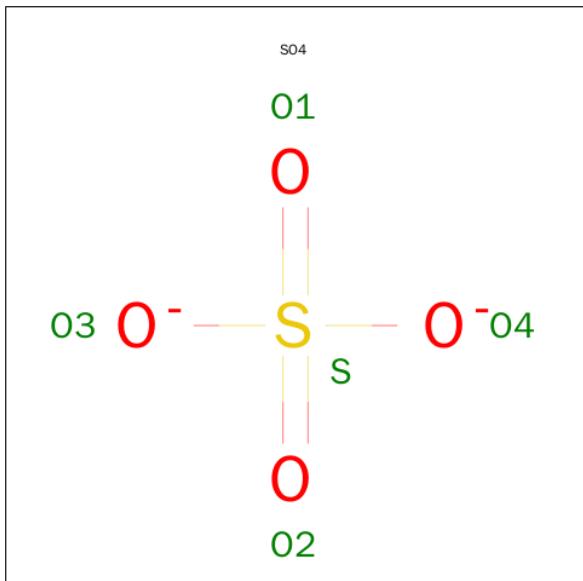
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	436	Total 436	O 436	0	0
4	B	498	Total 498	O 498	0	0

3 Residue-property plots ⓘ

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

Note EDS was not executed.

- Molecule 1: Lethal Factor precursor

Chain A:

- Molecule 1: Lethal Factor precursor

Chain B:
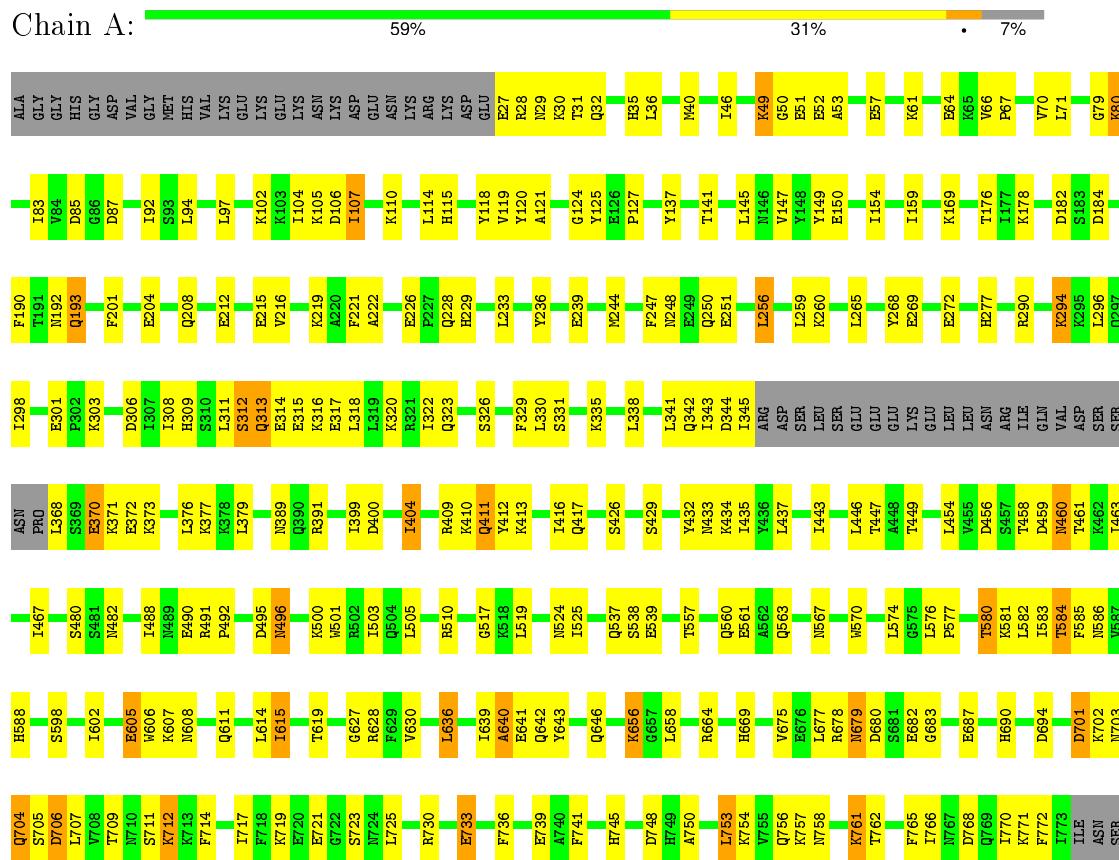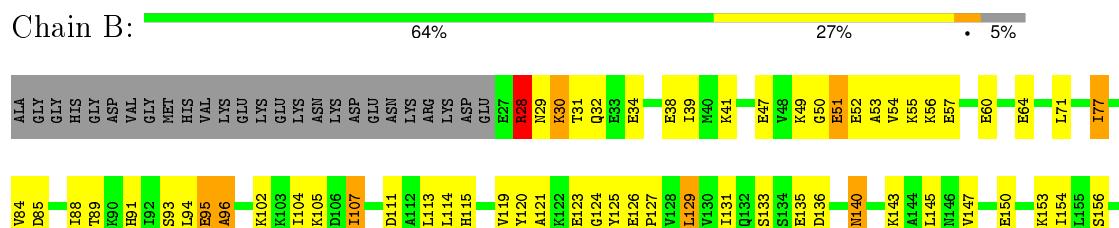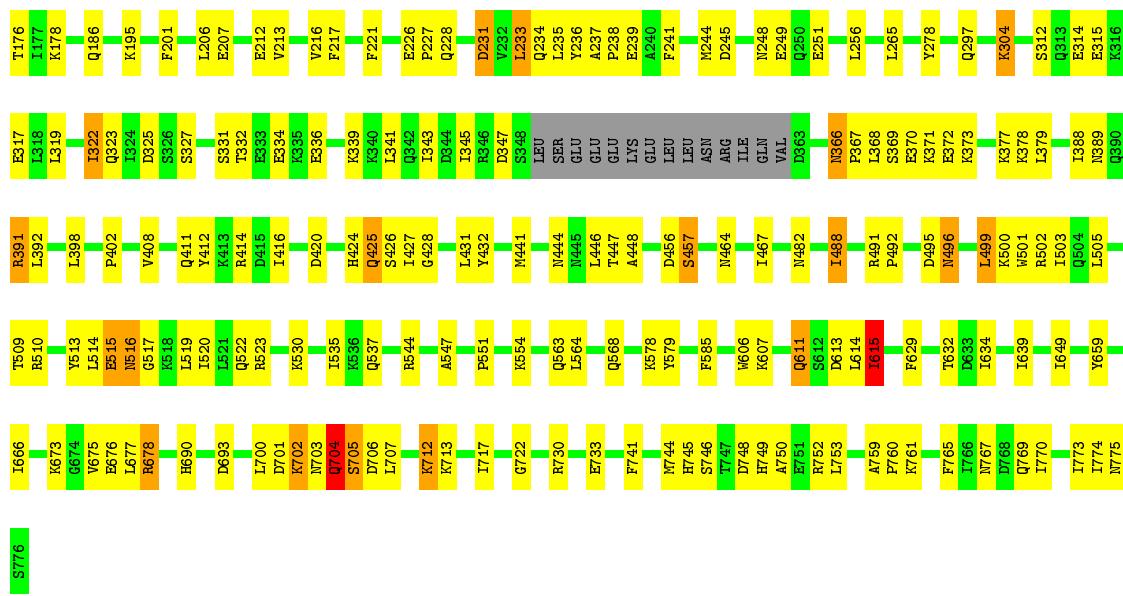
4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	96.20Å 137.46Å 98.55Å 90.00° 98.35° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30	Depositor
% Data completeness (in resolution range)	5.0 (15.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.229 , 0.261	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12924	wwPDB-VP
Average B, all atoms (Å^2)	44.0	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: ZN, 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	0.34	0/6053	0.57	1/8153 (0.0%)
1	B	0.36	1/6139 (0.0%)	0.59	2/8272 (0.0%)
All	All	0.35	1/12192 (0.0%)	0.58	3/16425 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	615	ILE	CG1-CD1	-5.50	1.12	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	615	ILE	CB-CG1-CD1	8.66	138.14	113.90
1	A	615	ILE	CB-CG1-CD1	-7.22	93.67	113.90
1	B	629	PHE	N-CA-C	-5.57	95.95	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	5947	0	5938	247	0
1	B	6031	0	5992	221	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	436	0	0	16	0
4	B	498	0	0	17	0
All	All	12924	0	11930	461	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 19.

All (461) 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:615:ILE:CG1	1:A:615:ILE:CD1	1.74	1.58
1:A:268:TYR:HB3	1:B:125:TYR:CE2	1.87	1.09
1:B:704:GLN:NE2	1:B:706:ASP:H	1.52	1.07
1:A:92:ILE:HD12	1:A:92:ILE:H	1.25	1.01
1:A:677:LEU:HD13	1:A:683:GLY:HA2	1.43	1.01
1:A:119:VAL:HG21	1:A:147:VAL:HG22	1.43	1.00
1:A:615:ILE:CB	1:A:615:ILE:CD1	2.39	1.00
1:B:304:LYS:HD3	1:B:304:LYS:H	1.27	0.96
1:A:615:ILE:HD13	1:A:615:ILE:HG21	1.46	0.96
1:B:510:ARG:H	1:B:522:GLN:HE21	1.05	0.95
1:B:632:THR:HG21	1:B:639:ILE:HD11	1.50	0.93
1:B:176:THR:HG21	1:B:239:GLU:HG3	1.53	0.89
1:A:268:TYR:HB3	1:B:125:TYR:HE2	1.38	0.88
1:B:712:LYS:HD2	1:B:712:LYS:H	1.35	0.88
1:B:606:TRP:CE2	1:B:615:ILE:HD12	2.10	0.86
1:A:107:ILE:HD11	1:A:219:LYS:HG3	1.56	0.85
1:A:567:ASN:HD21	1:A:583:ILE:H	1.19	0.85
1:B:366:ASN:H	1:B:367:PRO:HD2	1.42	0.84
1:A:636:LEU:HA	1:A:639:ILE:HD13	1.60	0.83
1:A:615:ILE:CD1	1:A:615:ILE:HG21	2.09	0.82
1:A:615:ILE:CG2	1:A:615:ILE:CD1	2.58	0.81
1:B:516:ASN:HD22	1:B:516:ASN:H	1.29	0.81
1:A:298:ILE:O	1:A:298:ILE:HD12	1.81	0.80
1:B:304:LYS:HD3	1:B:304:LYS:N	1.96	0.79
1:B:104:ILE:HG13	1:B:105:LYS:H	1.46	0.79
1:A:563:GLN:HE21	1:A:585:PHE:H	1.28	0.79
1:B:221:PHE:HD1	1:B:244:MET:HE1	1.48	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:GLN:HG2	1:B:195:LYS:HG2	1.65	0.78
1:B:516:ASN:ND2	1:B:516:ASN:H	1.80	0.78
1:A:615:ILE:HD13	1:A:615:ILE:CG2	2.14	0.78
1:B:370:GLU:HG2	1:B:371:LYS:HG3	1.66	0.78
1:B:516:ASN:HD22	1:B:516:ASN:N	1.80	0.77
1:A:714:PHE:HA	1:A:717:ILE:HD13	1.67	0.77
1:A:290:ARG:O	1:A:294:LYS:HE2	1.85	0.76
1:B:678:ARG:HB3	1:B:678:ARG:NH1	2.01	0.76
1:A:66:VAL:CG1	1:A:70:VAL:HG21	2.15	0.76
1:B:391:ARG:HG3	1:B:412:TYR:CD1	2.21	0.75
1:A:656:LYS:HE3	1:A:669:HIS:O	1.87	0.75
1:B:606:TRP:CZ2	1:B:615:ILE:HD12	2.22	0.74
1:B:501:TRP:HB3	1:B:503:ILE:HD11	1.68	0.74
1:B:322:ILE:HD13	1:B:323:GLN:N	2.02	0.74
1:A:176:THR:HG21	1:A:239:GLU:HG3	1.69	0.74
1:A:577:PRO:O	1:A:580:THR:HG22	1.89	0.73
1:A:563:GLN:NE2	1:A:585:PHE:H	1.87	0.72
1:B:713:LYS:HD2	1:B:765:PHE:HE1	1.52	0.72
1:B:233:LEU:HD23	1:B:237:ALA:HB3	1.69	0.72
1:B:611:GLN:HE22	1:B:613:ASP:HB2	1.54	0.72
1:B:510:ARG:H	1:B:522:GLN:NE2	1.85	0.72
1:B:412:TYR:O	1:B:416:ILE:HG12	1.91	0.71
1:A:107:ILE:HD13	1:A:107:ILE:O	1.89	0.71
1:A:176:THR:CG2	1:A:239:GLU:HG3	2.21	0.71
1:B:704:GLN:NE2	1:B:706:ASP:N	2.35	0.71
1:A:256:LEU:HD22	1:A:260:LYS:HE3	1.73	0.70
1:A:605:GLU:HG3	4:A:9361:HOH:O	1.91	0.70
1:A:761:LYS:HD3	1:A:761:LYS:C	2.12	0.69
1:A:391:ARG:NH1	1:A:404:ILE:HD12	2.06	0.69
1:B:212:GLU:O	1:B:216:VAL:HG23	1.92	0.69
1:B:717:ILE:HD12	1:B:761:LYS:HB3	1.73	0.69
1:A:500:LYS:HE2	1:A:537:GLN:HE22	1.57	0.69
1:B:713:LYS:HD2	1:B:765:PHE:CE1	2.27	0.69
1:A:308:ILE:HD12	1:A:345:ILE:HD11	1.75	0.68
1:B:107:ILE:HG21	1:B:145:LEU:HD12	1.74	0.68
1:B:693:ASP:OD2	1:B:707:LEU:HB3	1.93	0.68
1:B:398:LEU:HD23	4:B:9209:HOH:O	1.94	0.68
1:A:712:LYS:H	1:A:712:LYS:HE3	1.59	0.68
1:B:704:GLN:CD	1:B:706:ASP:H	1.97	0.67
1:B:121:ALA:HB1	1:B:154:ILE:HD11	1.75	0.67
1:B:369:SER:HB2	1:B:372:GLU:HG3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:563:GLN:NE2	1:B:585:PHE:H	1.91	0.66
1:A:614:LEU:HD22	1:A:770:ILE:HD12	1.77	0.66
1:B:123:GLU:HG2	1:B:124:GLY:H	1.60	0.66
1:A:268:TYR:HB3	1:B:125:TYR:CD2	2.31	0.66
1:A:717:ILE:HD12	1:A:717:ILE:H	1.60	0.66
1:B:121:ALA:HB2	1:B:150:GLU:HG3	1.77	0.65
1:A:712:LYS:HE3	1:A:712:LYS:N	2.10	0.65
1:A:443:ILE:HD13	1:A:454:LEU:HD22	1.78	0.65
1:B:304:LYS:CD	1:B:304:LYS:H	2.07	0.65
1:B:378:LYS:HE3	4:B:9364:HOH:O	1.96	0.65
1:A:119:VAL:CG2	1:A:147:VAL:HG22	2.21	0.65
1:A:679:ASN:ND2	1:A:682:GLU:H	1.95	0.65
1:A:404:ILE:HD13	1:A:404:ILE:H	1.61	0.65
1:A:317:GLU:O	1:A:320:LYS:HB3	1.97	0.65
1:A:102:LYS:HA	1:A:114:LEU:HD12	1.79	0.65
1:A:330:LEU:HB2	1:A:335:LYS:HE3	1.78	0.64
1:B:28:ARG:NH1	1:B:30:LYS:HB2	2.11	0.64
1:B:704:GLN:HE22	1:B:706:ASP:H	1.41	0.64
1:A:28:ARG:HG2	1:A:28:ARG:HH11	1.63	0.64
1:B:704:GLN:HE21	1:B:705:SER:N	1.96	0.64
1:A:500:LYS:HE2	1:A:537:GLN:NE2	2.13	0.64
1:B:749:HIS:HA	1:B:752:ARG:HD3	1.79	0.64
1:A:221:PHE:HD1	1:A:244:MET:HE1	1.63	0.64
1:B:107:ILE:O	1:B:107:ILE:HD13	1.99	0.63
1:A:28:ARG:HG3	1:A:29:ASN:H	1.62	0.63
1:A:107:ILE:HG21	1:A:145:LEU:HD12	1.81	0.62
1:A:639:ILE:O	1:A:640:ALA:CB	2.46	0.62
1:B:678:ARG:HB3	1:B:678:ARG:HH11	1.65	0.62
1:A:66:VAL:HG12	1:A:70:VAL:HG21	1.81	0.61
1:B:56:LYS:O	1:B:60:GLU:HG3	2.00	0.61
4:A:9302:HOH:O	1:B:491:ARG:HD3	2.01	0.61
1:A:66:VAL:HG11	1:A:70:VAL:HG21	1.83	0.60
1:B:488:ILE:HD13	1:B:517:GLY:O	2.00	0.60
1:A:717:ILE:N	1:A:717:ILE:HD12	2.16	0.60
1:B:319:LEU:HD23	1:B:345:ILE:HD11	1.82	0.60
1:B:722:GLY:HA3	1:B:730:ARG:HH11	1.64	0.60
1:B:119:VAL:HG23	1:B:131:ILE:HD13	1.82	0.60
1:B:510:ARG:N	1:B:522:GLN:HE21	1.89	0.60
1:B:104:ILE:HG13	1:B:105:LYS:N	2.16	0.60
1:A:322:ILE:HD11	1:A:376:LEU:HD11	1.84	0.60
1:B:178:LYS:HD2	1:B:201:PHE:CE1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:677:LEU:CD1	1:A:683:GLY:HA2	2.27	0.60
1:A:118:TYR:CD2	1:A:119:VAL:HG23	2.37	0.59
1:A:679:ASN:HD21	1:A:682:GLU:H	1.48	0.59
1:B:221:PHE:CD1	1:B:244:MET:HE1	2.34	0.59
1:A:311:LEU:HA	1:A:315:GLU:OE2	2.03	0.59
1:B:611:GLN:NE2	1:B:614:LEU:H	2.00	0.59
1:A:312:SER:N	1:A:316:LYS:HG3	2.18	0.59
1:A:607:LYS:HA	1:A:615:ILE:HD11	1.84	0.59
1:B:370:GLU:HG2	1:B:371:LYS:N	2.17	0.59
1:A:256:LEU:CD2	1:A:260:LYS:HE3	2.31	0.59
1:A:614:LEU:HD22	1:A:770:ILE:HG23	1.83	0.59
1:A:370:GLU:HG2	1:A:371:LYS:N	2.18	0.58
1:A:456:ASP:HB3	1:A:459:ASP:O	2.03	0.58
1:A:92:ILE:H	1:A:92:ILE:CD1	2.03	0.58
1:A:598:SER:O	1:A:602:ILE:HG13	2.03	0.58
1:A:717:ILE:HG23	1:A:761:LYS:HD2	1.86	0.58
1:B:245:ASP:O	1:B:249:GLU:HG2	2.04	0.58
1:B:29:ASN:HA	1:B:32:GLN:HB3	1.85	0.58
1:B:244:MET:HE3	1:B:248:ASN:HD21	1.68	0.58
1:A:46:ILE:N	1:A:46:ILE:HD12	2.18	0.58
1:A:608:ASN:HD22	1:A:608:ASN:N	2.00	0.58
1:A:753:LEU:O	1:A:756:GLN:HB3	2.03	0.57
1:A:83:ILE:N	1:A:83:ILE:HD12	2.19	0.57
1:A:277:HIS:CD2	1:A:429:SER:HB2	2.39	0.57
1:A:303:LYS:HE3	1:A:306:ASP:OD1	2.04	0.57
1:B:704:GLN:OE1	1:B:706:ASP:C	2.43	0.57
1:B:28:ARG:H	1:B:28:ARG:HD3	1.70	0.57
1:A:314:GLU:O	1:A:318:LEU:HG	2.04	0.57
1:A:204:GLU:O	1:A:208:GLN:HG2	2.05	0.57
1:A:244:MET:CE	1:A:248:ASN:HD21	2.18	0.57
1:B:304:LYS:HD2	4:B:9411:HOH:O	2.04	0.57
1:A:268:TYR:CB	1:B:125:TYR:HE2	2.15	0.56
1:B:733:GLU:HG2	4:B:9233:HOH:O	2.05	0.56
1:B:244:MET:CE	1:B:248:ASN:HD21	2.18	0.56
1:B:28:ARG:HH12	1:B:30:LYS:HD2	1.71	0.56
1:B:456:ASP:O	1:B:457:SER:CB	2.53	0.56
1:A:94:LEU:HB3	1:A:97:LEU:HD12	1.87	0.56
1:A:584:THR:HG23	1:A:630:VAL:HG22	1.88	0.56
1:B:39:ILE:HG21	1:B:71:LEU:HB3	1.87	0.56
1:B:456:ASP:O	1:B:457:SER:HB3	2.06	0.56
1:A:27:GLU:N	1:A:30:LYS:HB3	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:717:ILE:CG2	1:A:761:LYS:HD2	2.36	0.56
1:B:60:GLU:O	1:B:64:GLU:HB2	2.06	0.56
1:B:523:ARG:HG2	4:B:9025:HOH:O	2.06	0.56
1:A:757:LYS:HD3	4:A:9240:HOH:O	2.06	0.56
1:A:614:LEU:CD2	1:A:770:ILE:HD12	2.35	0.56
1:A:28:ARG:HG3	1:A:29:ASN:N	2.21	0.56
1:A:184:ASP:HB3	1:A:236:TYR:HB3	1.87	0.56
1:A:212:GLU:O	1:A:216:VAL:HG23	2.06	0.56
1:B:366:ASN:H	1:B:367:PRO:CD	2.16	0.56
1:A:712:LYS:H	1:A:712:LYS:CE	2.18	0.56
1:A:741:PHE:O	1:A:745:HIS:HD2	1.89	0.55
1:A:449:THR:HG21	4:A:9251:HOH:O	2.05	0.55
1:A:272:GLU:HG3	1:B:125:TYR:CE1	2.41	0.55
4:A:9170:HOH:O	1:B:124:GLY:HA2	2.06	0.55
1:B:391:ARG:HG3	1:B:412:TYR:CE1	2.41	0.55
1:A:495:ASP:OD2	1:B:495:ASP:HB2	2.07	0.55
1:A:488:ILE:HD13	1:A:517:GLY:O	2.07	0.55
1:B:733:GLU:CD	1:B:733:GLU:H	2.09	0.54
1:A:178:LYS:HB3	1:A:190:PHE:HE1	1.71	0.54
1:B:431:LEU:HG	4:B:9306:HOH:O	2.06	0.54
1:A:643:TYR:HA	1:A:646:GLN:HG3	1.90	0.54
1:B:28:ARG:O	1:B:32:GLN:HB2	2.07	0.54
1:A:460:ASN:HD22	1:A:461:THR:N	2.05	0.54
1:A:247:PHE:HA	1:A:251:GLU:HB2	1.89	0.54
1:A:615:ILE:O	1:A:619:THR:HG23	2.08	0.54
1:B:704:GLN:NE2	1:B:705:SER:N	2.55	0.54
1:B:693:ASP:CG	1:B:707:LEU:HB3	2.29	0.54
1:A:496:ASN:C	1:A:496:ASN:HD22	2.10	0.54
1:B:368:LEU:HB2	1:B:373:LYS:HG2	1.90	0.53
1:A:524:ASN:ND2	4:A:9004:HOH:O	2.41	0.53
1:A:322:ILE:HA	1:A:368:LEU:HD13	1.89	0.53
1:A:748:ASP:OD2	1:A:750:ALA:HB3	2.09	0.53
1:A:733:GLU:CD	1:A:733:GLU:H	2.12	0.53
1:A:154:ILE:HG22	1:A:159:ILE:HD13	1.91	0.53
1:B:31:THR:HA	1:B:34:GLU:HB3	1.89	0.53
1:A:712:LYS:CD	1:A:712:LYS:H	2.21	0.53
1:A:611:GLN:NE2	1:A:770:ILE:HG21	2.24	0.53
1:B:722:GLY:HA3	1:B:730:ARG:NH1	2.24	0.53
1:A:31:THR:O	1:A:35:HIS:HB2	2.08	0.53
1:A:404:ILE:N	1:A:404:ILE:HD13	2.24	0.52
1:A:570:TRP:O	1:A:574:LEU:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:ASP:HA	1:A:707:LEU:HD23	1.91	0.52
1:A:733:GLU:CD	1:A:733:GLU:N	2.63	0.52
1:A:272:GLU:HG3	1:B:125:TYR:CD1	2.44	0.52
1:B:578:LYS:O	1:B:579:TYR:HB2	2.10	0.52
1:B:392:LEU:HD11	1:B:416:ILE:HD12	1.92	0.52
1:B:38:GLU:O	1:B:41:LYS:HB3	2.09	0.52
1:B:312:SER:OG	1:B:315:GLU:HG3	2.10	0.52
1:A:491:ARG:HB3	1:A:492:PRO:HD2	1.92	0.52
1:A:66:VAL:HG12	1:A:70:VAL:CG2	2.39	0.51
1:A:488:ILE:HD13	1:A:517:GLY:C	2.31	0.51
1:A:107:ILE:HG21	1:A:145:LEU:CD1	2.40	0.51
1:A:322:ILE:HD12	1:A:372:GLU:OE1	2.10	0.51
1:B:114:LEU:HD21	1:B:120:TYR:HB2	1.92	0.51
1:A:104:ILE:HG22	1:A:105:LYS:N	2.25	0.51
1:B:47:GLU:O	1:B:84:VAL:HG23	2.11	0.51
1:A:577:PRO:O	1:A:580:THR:CG2	2.58	0.51
1:B:126:GLU:N	1:B:127:PRO:CD	2.72	0.51
1:B:206:LEU:O	1:B:206:LEU:HD13	2.11	0.51
1:A:413:LYS:O	1:A:417:GLN:HG3	2.11	0.51
1:B:317:GLU:HB2	4:B:9189:HOH:O	2.10	0.51
1:A:766:ILE:O	1:A:770:ILE:HG12	2.11	0.51
1:B:140:ASN:ND2	1:B:143:LYS:NZ	2.59	0.51
1:A:49:LYS:HD2	1:A:51:GLU:OE1	2.11	0.50
1:A:329:PHE:HE2	1:A:377:LYS:HA	1.75	0.50
1:B:121:ALA:HB1	1:B:154:ILE:CD1	2.41	0.50
1:A:627:GLY:HA3	1:A:664:ARG:O	2.12	0.50
1:A:28:ARG:CG	1:A:29:ASN:H	2.25	0.50
1:B:759:ALA:N	1:B:760:PRO:HD3	2.26	0.50
1:A:368:LEU:HD22	1:A:372:GLU:CD	2.32	0.50
1:A:717:ILE:H	1:A:717:ILE:CD1	2.23	0.50
1:A:426:SER:HA	1:A:510:ARG:HA	1.94	0.50
1:A:725:LEU:HD12	1:A:736:PHE:CE1	2.47	0.50
1:B:702:LYS:N	1:B:702:LYS:HD2	2.26	0.50
1:A:368:LEU:HB3	1:A:370:GLU:OE1	2.11	0.50
1:A:330:LEU:HD13	1:A:338:LEU:HD12	1.94	0.49
1:A:221:PHE:CD1	1:A:244:MET:HE1	2.46	0.49
1:A:704:GLN:NE2	1:A:705:SER:HB3	2.27	0.49
1:B:611:GLN:HE22	1:B:613:ASP:CB	2.23	0.49
1:A:433:ASN:O	1:A:435:ILE:HD12	2.12	0.49
1:A:70:VAL:CG2	1:A:71:LEU:N	2.75	0.49
1:A:606:TRP:CH2	1:A:615:ILE:HG23	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:LEU:O	1:B:322:ILE:HG22	2.12	0.49
1:A:341:LEU:O	1:A:345:ILE:HG12	2.12	0.49
1:A:322:ILE:HA	1:A:368:LEU:CD1	2.42	0.49
1:B:373:LYS:O	1:B:377:LYS:HG3	2.12	0.49
1:B:500:LYS:HD3	1:B:537:GLN:HE22	1.77	0.49
1:A:576:LEU:HB3	1:A:580:THR:HG21	1.95	0.49
1:A:322:ILE:HG13	1:A:368:LEU:HD13	1.93	0.49
1:B:47:GLU:OE1	1:B:91:HIS:HE1	1.95	0.49
1:B:441:MET:O	1:B:499:LEU:HB2	2.13	0.49
1:A:723:SER:HB3	1:A:730:ARG:NH1	2.27	0.49
1:A:57:GLU:O	1:A:61:LYS:HG2	2.12	0.49
1:B:278:TYR:HE2	1:B:425:GLN:HB3	1.76	0.49
1:A:70:VAL:HG23	1:A:71:LEU:N	2.27	0.49
1:B:659:TYR:HD1	1:B:666:ILE:HD13	1.77	0.49
1:B:150:GLU:OE2	1:B:153:LYS:NZ	2.46	0.48
1:A:707:LEU:HB3	1:A:709:THR:HG22	1.95	0.48
1:A:432:TYR:CD1	1:A:435:ILE:HD11	2.48	0.48
1:B:176:THR:CG2	1:B:239:GLU:HG3	2.34	0.48
1:A:537:GLN:NE2	4:A:9115:HOH:O	2.46	0.48
1:B:34:GLU:O	1:B:38:GLU:HG3	2.13	0.48
1:B:54:VAL:HA	1:B:57:GLU:OE2	2.12	0.48
1:B:129:LEU:HD11	1:B:131:ILE:HD11	1.96	0.48
1:B:113:LEU:HD22	1:B:113:LEU:N	2.28	0.48
1:A:331:SER:O	1:A:335:LYS:HG2	2.14	0.48
1:A:28:ARG:HG3	1:A:29:ASN:OD1	2.13	0.48
1:A:159:ILE:HD12	1:A:159:ILE:N	2.27	0.48
1:B:85:ASP:HB3	1:B:133:SER:OG	2.12	0.48
1:A:49:LYS:HB2	1:A:51:GLU:OE1	2.13	0.48
1:A:329:PHE:CE2	1:A:377:LYS:HA	2.49	0.48
1:B:551:PRO:HD2	1:B:554:LYS:HE3	1.95	0.48
1:B:632:THR:OG1	1:B:634:ILE:HG12	2.14	0.48
1:B:607:LYS:HE2	4:B:9155:HOH:O	2.14	0.48
1:A:701:ASP:OD1	1:A:704:GLN:HB3	2.13	0.48
1:A:67:PRO:O	1:A:70:VAL:HG22	2.13	0.47
1:A:61:LYS:O	1:A:64:GLU:HB3	2.12	0.47
1:A:656:LYS:HE2	1:A:680:ASP:OD2	2.13	0.47
1:A:244:MET:HE3	1:A:248:ASN:HD21	1.77	0.47
1:A:705:SER:O	1:A:706:ASP:HB2	2.14	0.47
1:A:104:ILE:CG2	1:A:105:LYS:N	2.77	0.47
1:B:89:THR:O	1:B:89:THR:HG22	2.15	0.47
1:B:331:SER:OG	1:B:334:GLU:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:608:ASN:N	1:A:608:ASN:ND2	2.62	0.47
1:B:143:LYS:O	1:B:147:VAL:HG23	2.14	0.47
1:B:703:ASN:O	1:B:704:GLN:CB	2.62	0.47
1:B:178:LYS:HD2	1:B:201:PHE:CZ	2.50	0.47
1:A:154:ILE:O	1:A:159:ILE:HD13	2.15	0.47
1:B:206:LEU:HD13	1:B:206:LEU:C	2.35	0.47
1:B:408:VAL:HA	1:B:411:GLN:HG2	1.97	0.47
1:B:77:ILE:O	1:B:77:ILE:HG23	2.15	0.47
1:B:125:TYR:CD1	1:B:125:TYR:N	2.83	0.47
1:B:706:ASP:O	1:B:707:LEU:HD23	2.15	0.47
1:A:679:ASN:HD22	1:A:679:ASN:H	1.63	0.47
1:A:29:ASN:HA	1:A:32:GLN:HB2	1.97	0.47
1:B:564:LEU:O	1:B:568:GLN:HG3	2.14	0.47
1:B:304:LYS:HA	1:B:341:LEU:HD21	1.97	0.47
1:B:741:PHE:O	1:B:745:HIS:HD2	1.98	0.47
1:B:119:VAL:HG23	1:B:131:ILE:CD1	2.45	0.47
1:A:611:GLN:HE22	1:A:770:ILE:HG21	1.80	0.46
1:B:52:GLU:HG3	1:B:52:GLU:O	2.14	0.46
1:B:675:VAL:O	1:B:676:GLU:HB2	2.15	0.46
1:A:28:ARG:HG2	1:A:28:ARG:NH1	2.26	0.46
1:B:535:ILE:HD13	1:B:544:ARG:HB2	1.96	0.46
1:B:368:LEU:HA	4:B:9278:HOH:O	2.14	0.46
1:B:319:LEU:HD23	1:B:345:ILE:CD1	2.44	0.46
1:A:411:GLN:HE21	1:A:411:GLN:HA	1.80	0.46
1:A:721:GLU:OE1	1:A:761:LYS:HB3	2.15	0.46
1:A:454:LEU:HG	1:A:463:ILE:HD12	1.97	0.46
1:A:560:GLN:HG2	4:A:9041:HOH:O	2.16	0.46
1:B:496:ASN:C	1:B:496:ASN:HD22	2.18	0.46
1:B:515:GLU:O	1:B:515:GLU:CD	2.54	0.46
1:A:501:TRP:HB3	1:A:503:ILE:HD11	1.97	0.46
1:A:656:LYS:O	1:A:656:LYS:HD3	2.16	0.46
1:A:557:THR:O	1:A:561:GLU:HG3	2.15	0.46
1:B:402:PRO:O	1:B:649:ILE:HD12	2.16	0.46
1:A:36:LEU:O	1:A:40:MET:HG2	2.15	0.46
1:B:95:GLU:O	1:B:96:ALA:HB2	2.16	0.46
1:B:690:HIS:O	1:B:693:ASP:HB3	2.15	0.46
1:B:388:ILE:HG23	1:B:416:ILE:HD11	1.97	0.46
1:A:322:ILE:HD13	1:A:376:LEU:HD21	1.98	0.46
1:B:464:ASN:HB3	4:B:9084:HOH:O	2.15	0.46
1:A:124:GLY:O	1:A:127:PRO:HD3	2.16	0.46
1:A:434:LYS:HB3	1:A:434:LYS:NZ	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:ILE:HG23	1:B:416:ILE:CD1	2.46	0.45
1:A:323:GLN:HB3	1:A:326:SER:OG	2.15	0.45
1:A:193:GLN:HE21	1:A:193:GLN:HA	1.80	0.45
1:A:480:SER:HB3	1:A:525:ILE:HB	1.98	0.45
1:B:673:LYS:NZ	1:B:677:LEU:O	2.49	0.45
1:B:530:LYS:NZ	4:B:9092:HOH:O	2.49	0.45
1:B:370:GLU:HG2	1:B:371:LYS:H	1.80	0.45
1:B:502:ARG:C	1:B:503:ILE:HD13	2.37	0.45
1:B:420:ASP:OD1	1:B:523:ARG:HD3	2.17	0.45
1:A:169:LYS:HB3	4:A:9056:HOH:O	2.16	0.45
1:B:426:SER:HA	1:B:510:ARG:HA	1.99	0.45
1:B:611:GLN:HE21	1:B:614:LEU:H	1.65	0.45
1:A:433:ASN:O	1:A:435:ILE:CD1	2.65	0.45
1:A:269:GLU:HB2	4:A:9290:HOH:O	2.17	0.45
1:B:389:ASN:OD1	1:B:482:ASN:HB2	2.17	0.45
1:B:88:ILE:O	1:B:94:LEU:HD12	2.17	0.45
1:A:538:SER:O	1:A:539:GLU:HB2	2.17	0.45
1:A:758:ASN:HB3	4:A:9183:HOH:O	2.16	0.45
1:A:87:ASP:OD1	1:A:115:HIS:HB2	2.17	0.45
1:B:427:ILE:O	1:B:428:GLY:C	2.55	0.45
1:A:701:ASP:C	1:A:703:ASN:H	2.20	0.44
1:A:244:MET:HE3	1:A:248:ASN:ND2	2.32	0.44
1:A:467:ILE:HD12	1:A:467:ILE:N	2.32	0.44
1:B:28:ARG:C	1:B:30:LYS:H	2.20	0.44
1:A:768:ASP:O	1:A:771:LYS:HB3	2.17	0.44
1:A:141:THR:HG21	1:A:228:GLN:HG3	1.99	0.44
1:A:765:PHE:HD2	1:A:766:ILE:HD12	1.82	0.44
1:B:700:LEU:O	1:B:701:ASP:HB3	2.18	0.44
1:B:769:GLN:O	1:B:773:ILE:HD13	2.18	0.44
1:A:149:TYR:HA	1:A:222:ALA:HB2	1.98	0.44
1:B:327:SER:HA	4:B:9214:HOH:O	2.17	0.44
1:A:121:ALA:HB2	1:A:150:GLU:HG3	1.98	0.44
1:A:584:THR:CG2	1:A:630:VAL:HG22	2.48	0.44
1:A:687:GLU:O	1:A:690:HIS:HB2	2.17	0.44
1:B:505:LEU:HD22	1:B:509:THR:HG21	1.99	0.44
1:B:244:MET:HE3	1:B:248:ASN:ND2	2.32	0.44
1:A:679:ASN:ND2	1:A:682:GLU:HB2	2.32	0.44
1:B:91:HIS:CD2	1:B:93:SER:H	2.36	0.44
1:A:409:ARG:HD2	4:A:9119:HOH:O	2.17	0.44
1:B:125:TYR:N	1:B:125:TYR:HD1	2.16	0.44
1:A:338:LEU:HD23	1:A:341:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:444:ASN:HD22	1:B:448:ALA:HA	1.82	0.44
1:A:412:TYR:O	1:A:416:ILE:HG13	2.18	0.44
1:B:226:GLU:OE1	1:B:228:GLN:HB2	2.18	0.43
1:B:414:ARG:NH2	4:B:9146:HOH:O	2.50	0.43
1:B:704:GLN:CD	1:B:706:ASP:N	2.67	0.43
1:B:611:GLN:NE2	1:B:613:ASP:HB2	2.29	0.43
1:A:675:VAL:HG22	1:A:675:VAL:O	2.18	0.43
1:B:744:MET:C	1:B:752:ARG:HG2	2.38	0.43
1:B:366:ASN:N	1:B:367:PRO:HD2	2.20	0.43
1:B:206:LEU:HD23	1:B:213:VAL:HG21	2.00	0.43
1:A:373:LYS:HD2	1:A:377:LYS:HE3	2.00	0.43
1:B:713:LYS:O	1:B:717:ILE:HG12	2.18	0.43
1:A:490:GLU:OE2	1:A:500:LYS:HE3	2.18	0.43
1:B:444:ASN:ND2	1:B:448:ALA:HA	2.34	0.43
1:B:704:GLN:NE2	1:B:704:GLN:C	2.72	0.43
1:B:370:GLU:N	1:B:370:GLU:OE2	2.49	0.43
1:A:294:LYS:NZ	4:A:9167:HOH:O	2.51	0.43
1:B:678:ARG:HB3	1:B:678:ARG:CZ	2.48	0.43
1:B:339:LYS:O	1:B:343:ILE:HG12	2.17	0.43
1:B:297:GLN:NE2	1:B:514:LEU:HD13	2.33	0.43
1:A:639:ILE:HG22	1:A:641:GLU:H	1.84	0.43
1:B:491:ARG:HB3	1:B:492:PRO:HD2	2.00	0.43
1:A:370:GLU:N	1:A:370:GLU:OE1	2.44	0.43
1:B:408:VAL:HA	1:B:411:GLN:CG	2.49	0.43
1:B:212:GLU:HG2	4:B:9135:HOH:O	2.18	0.43
1:B:712:LYS:CD	1:B:712:LYS:H	2.07	0.42
1:B:28:ARG:HH11	1:B:30:LYS:HB2	1.83	0.42
1:A:741:PHE:O	1:A:745:HIS:CD2	2.72	0.42
1:B:767:ASN:HA	1:B:767:ASN:HD22	1.59	0.42
1:B:513:TYR:HA	1:B:519:LEU:HD23	2.01	0.42
1:A:639:ILE:O	1:A:640:ALA:HB3	2.20	0.42
1:A:159:ILE:CD1	1:A:159:ILE:N	2.82	0.42
1:A:49:LYS:HG3	1:A:85:ASP:OD1	2.19	0.42
1:A:226:GLU:HB3	1:A:229:HIS:HB2	2.00	0.42
1:B:55:LYS:HD3	1:B:133:SER:HB2	2.01	0.42
1:A:719:LYS:HE2	1:A:719:LYS:N	2.35	0.42
1:B:156:SER:HB2	1:B:217:PHE:CD2	2.54	0.42
1:A:410:LYS:HG3	4:A:9333:HOH:O	2.18	0.42
1:A:119:VAL:HG12	1:A:120:TYR:N	2.35	0.42
1:A:182:ASP:OD1	1:A:184:ASP:N	2.51	0.42
1:A:389:ASN:OD1	1:A:482:ASN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLY:O	1:A:80:LYS:HD2	2.19	0.42
1:A:639:ILE:O	1:A:640:ALA:HB2	2.19	0.42
1:B:748:ASP:OD1	1:B:750:ALA:HB3	2.20	0.42
1:B:237:ALA:N	1:B:238:PRO:HD3	2.35	0.42
1:B:746:SER:O	1:B:752:ARG:HD2	2.19	0.42
1:A:309:HIS:O	1:A:309:HIS:ND1	2.52	0.42
1:B:775:ASN:HA	4:B:9476:HOH:O	2.20	0.42
1:B:126:GLU:N	1:B:127:PRO:HD3	2.34	0.42
1:B:234:GLN:HB2	1:B:241:PHE:CD2	2.55	0.42
1:B:503:ILE:HD12	1:B:547:ALA:HB3	2.01	0.41
1:A:368:LEU:N	1:A:368:LEU:HD12	2.34	0.41
1:A:178:LYS:HD2	1:A:201:PHE:CE1	2.55	0.41
1:A:581:LYS:HE3	1:A:628:ARG:HH21	1.84	0.41
1:A:106:ASP:OD1	1:A:110:LYS:HE3	2.20	0.41
1:B:231:ASP:O	1:B:235:LEU:HB2	2.20	0.41
1:A:70:VAL:HG23	1:A:71:LEU:HD12	2.01	0.41
1:B:611:GLN:NE2	1:B:613:ASP:N	2.69	0.41
1:A:679:ASN:HD22	1:A:679:ASN:N	2.17	0.41
1:A:723:SER:HB3	1:A:730:ARG:HH12	1.85	0.41
1:B:49:LYS:HD2	1:B:50:GLY:N	2.35	0.41
1:A:342:GLN:C	1:A:344:ASP:H	2.24	0.41
1:A:640:ALA:C	1:A:642:GLN:N	2.73	0.41
1:A:460:ASN:C	1:A:460:ASN:ND2	2.73	0.41
1:B:235:LEU:HD23	1:B:236:TYR:CE2	2.55	0.41
1:A:678:ARG:HD3	4:A:9226:HOH:O	2.20	0.41
1:B:704:GLN:HE21	1:B:704:GLN:C	2.24	0.41
1:A:313:GLN:HB2	4:A:9248:HOH:O	2.20	0.41
1:B:332:THR:HG22	1:B:336:GLU:OE2	2.20	0.41
1:B:388:ILE:HD13	1:B:412:TYR:CD2	2.56	0.41
1:B:388:ILE:HD13	1:B:412:TYR:HD2	1.86	0.41
1:B:457:SER:CA	4:B:9182:HOH:O	2.68	0.41
1:B:136:ASP:O	1:B:140:ASN:N	2.54	0.41
1:A:49:LYS:H	1:A:49:LYS:HG3	1.69	0.41
1:B:278:TYR:CE2	1:B:425:GLN:HB3	2.54	0.41
1:B:703:ASN:O	1:B:704:GLN:HB2	2.20	0.41
1:B:488:ILE:HD13	1:B:517:GLY:C	2.40	0.41
1:B:424:HIS:HA	1:B:510:ARG:HD2	2.03	0.41
1:A:586:ASN:OD1	1:A:588:HIS:CE1	2.74	0.41
1:A:92:ILE:HD12	1:A:92:ILE:N	2.10	0.41
1:A:711:SER:HA	1:A:712:LYS:HE3	2.03	0.41
1:B:121:ALA:CB	1:B:150:GLU:HG3	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLU:CD	1:A:51:GLU:H	2.24	0.41
1:A:606:TRP:CZ2	1:A:615:ILE:HG23	2.56	0.41
1:A:28:ARG:CG	1:A:29:ASN:N	2.82	0.41
1:B:457:SER:HA	4:B:9182:HOH:O	2.21	0.41
1:A:31:THR:O	1:A:31:THR:HG22	2.21	0.41
1:B:107:ILE:HG21	1:B:145:LEU:CD1	2.45	0.40
1:A:94:LEU:O	1:A:97:LEU:HB2	2.21	0.40
1:B:226:GLU:OE2	1:B:227:PRO:HD2	2.21	0.40
1:A:739:GLU:HA	1:A:739:GLU:OE1	2.21	0.40
1:B:770:ILE:O	1:B:774:ILE:HG13	2.22	0.40
1:B:54:VAL:HA	1:B:57:GLU:HG2	2.03	0.40
1:A:501:TRP:CE3	1:A:503:ILE:HD11	2.56	0.40
1:A:719:LYS:HE2	1:A:719:LYS:CA	2.52	0.40
1:A:437:LEU:HD11	1:A:519:LEU:HD12	2.03	0.40
1:A:219:LYS:HE3	1:A:219:LYS:HB2	1.94	0.40
1:A:463:ILE:HD13	1:A:463:ILE:HA	1.93	0.40
1:A:399:ILE:HD12	1:A:400:ASP:N	2.36	0.40
1:A:762:THR:HG23	1:A:766:ILE:HD13	2.02	0.40
1:A:226:GLU:OE1	1:A:228:GLN:HB2	2.22	0.40
1:B:467:ILE:HD12	1:B:467:ILE:N	2.36	0.40
1:B:611:GLN:HE22	1:B:613:ASP:CA	2.35	0.40
1:B:456:ASP:HA	1:B:464:ASN:OD1	2.22	0.40
1:A:36:LEU:O	1:A:36:LEU:HD23	2.22	0.40
1:A:754:LYS:HB3	1:A:754:LYS:HE2	1.97	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	721/776 (93%)	670 (93%)	38 (5%)	13 (2%)	11	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	732/776 (94%)	685 (94%)	35 (5%)	12 (2%)	12	11
All	All	1453/1552 (94%)	1355 (93%)	73 (5%)	25 (2%)	11	10

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
1	A	313	GLN
1	A	640	ALA
1	B	28	ARG
1	B	96	ALA
1	B	704	GLN
1	A	701	ASP
1	A	706	ASP
1	A	772	PHE
1	B	30	LYS
1	B	51	GLU
1	B	140	ASN
1	B	251	GLU
1	B	366	ASN
1	B	457	SER
1	A	53	ALA
1	A	250	GLN
1	A	702	LYS
1	B	53	ALA
1	A	52	GLU
1	A	312	SER
1	B	325	ASP
1	B	705	SER
1	A	343	ILE
1	A	50	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	660/710 (93%)	623 (94%)	37 (6%)	26	35
1	B	669/710 (94%)	631 (94%)	38 (6%)	25	34
All	All	1329/1420 (94%)	1254 (94%)	75 (6%)	26	35

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	LYS
1	A	107	ILE
1	A	125	TYR
1	A	137	TYR
1	A	192	ASN
1	A	193	GLN
1	A	215	GLU
1	A	233	LEU
1	A	256	LEU
1	A	259	LEU
1	A	265	LEU
1	A	294	LYS
1	A	296	LEU
1	A	301	GLU
1	A	370	GLU
1	A	379	LEU
1	A	404	ILE
1	A	411	GLN
1	A	446	LEU
1	A	447	THR
1	A	458	THR
1	A	460	ASN
1	A	496	ASN
1	A	505	LEU
1	A	580	THR
1	A	582	LEU
1	A	584	THR
1	A	605	GLU
1	A	636	LEU
1	A	656	LYS
1	A	658	LEU
1	A	679	ASN
1	A	704	GLN
1	A	712	LYS
1	A	733	GLU

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Mol	Chain	Res	Type
1	A	753	LEU
1	A	761	LYS
1	B	28	ARG
1	B	51	GLU
1	B	77	ILE
1	B	95	GLU
1	B	102	LYS
1	B	107	ILE
1	B	111	ASP
1	B	115	HIS
1	B	129	LEU
1	B	135	GLU
1	B	207	GLU
1	B	231	ASP
1	B	233	LEU
1	B	256	LEU
1	B	265	LEU
1	B	304	LYS
1	B	314	GLU
1	B	322	ILE
1	B	347	ASP
1	B	379	LEU
1	B	391	ARG
1	B	425	GLN
1	B	432	TYR
1	B	446	LEU
1	B	447	THR
1	B	488	ILE
1	B	496	ASN
1	B	499	LEU
1	B	515	GLU
1	B	516	ASN
1	B	520	ILE
1	B	611	GLN
1	B	615	ILE
1	B	678	ARG
1	B	702	LYS
1	B	704	GLN
1	B	712	LYS
1	B	753	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	164	ASN
1	A	165	GLN
1	A	193	GLN
1	A	197	HIS
1	A	209	ASN
1	A	214	GLN
1	A	242	ASN
1	A	248	ASN
1	A	276	GLN
1	A	277	HIS
1	A	279	GLN
1	A	297	GLN
1	A	390	GLN
1	A	393	GLN
1	A	411	GLN
1	A	440	ASN
1	A	445	ASN
1	A	460	ASN
1	A	496	ASN
1	A	524	ASN
1	A	537	GLN
1	A	563	GLN
1	A	567	ASN
1	A	571	ASN
1	A	588	HIS
1	A	589	ASN
1	A	608	ASN
1	A	611	GLN
1	A	652	GLN
1	A	679	ASN
1	A	704	GLN
1	A	710	ASN
1	A	745	HIS
1	A	767	ASN
1	B	91	HIS
1	B	117	HIS
1	B	140	ASN
1	B	164	ASN
1	B	165	GLN
1	B	186	GLN
1	B	193	GLN
1	B	197	HIS
1	B	214	GLN

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Mol	Chain	Res	Type
1	B	242	ASN
1	B	248	ASN
1	B	279	GLN
1	B	297	GLN
1	B	323	GLN
1	B	390	GLN
1	B	411	GLN
1	B	424	HIS
1	B	440	ASN
1	B	444	ASN
1	B	445	ASN
1	B	496	ASN
1	B	504	GLN
1	B	516	ASN
1	B	522	GLN
1	B	524	ASN
1	B	533	GLN
1	B	537	GLN
1	B	563	GLN
1	B	571	ASN
1	B	589	ASN
1	B	608	ASN
1	B	609	ASN
1	B	611	GLN
1	B	638	ASN
1	B	704	GLN
1	B	745	HIS
1	B	756	GLN
1	B	767	ASN
1	B	769	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	#$|Z| > 2$
2	SO4	A	777	-	4,4,4	0.08	0	6,6,6	0.12	0
2	SO4	B	777	-	4,4,4	0.19	0	6,6,6	0.08	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	777	-	-	0/0/0/0	0/0/0/0
2	SO4	B	777	-	-	0/0/0/0	0/0/0/0

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.

No monomer is involved in short contacts.

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)

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates (i)

EDS was not executed - this section will therefore be empty.

6.4 Ligands (i)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers (i)

EDS was not executed - this section will therefore be empty.