Full wwPDB X-ray Structure Validation Report

Jan 31, 2016 – 09:50 PM GMT

PDB ID	:	1QPO
Title	:	Quinolinate Phosphoribosyl Transferase (QAPRTase) Apo-Enzyme from Mycobacterium Tuberculosis
Authors	:	Sharma, V.; Grubmeyer, C.; Sacchettini, J.C.; TB Structural Genomics Consortium (TBSGC)
Deposited on	:	1998-11-21
Resolution	:	2.40 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 (i) symbol.

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

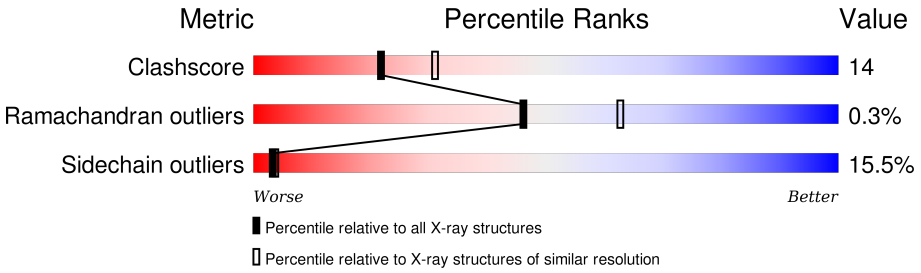
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.40 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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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	284	67% 26% 7%
1	B	284	69% 25% 7%
1	C	284	69% 25% 7%
1	D	284	70% 24% 6%
1	E	284	68% 25% 6%
1	F	284	69% 24% 7%

2 Entry composition (i)

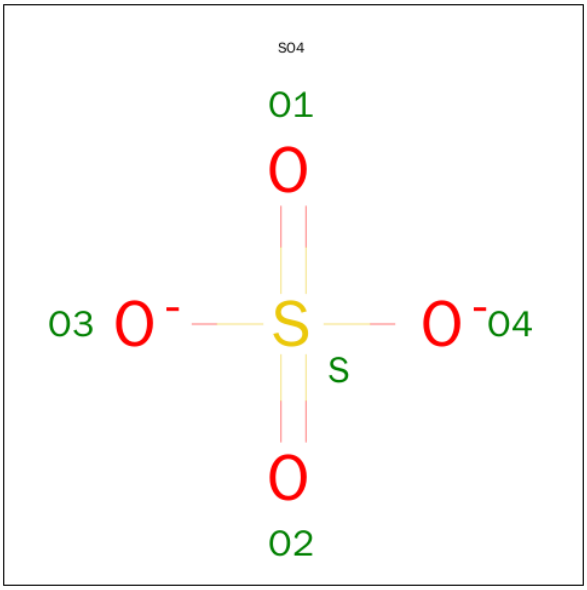
There are 3 unique types of molecules in this entry. The entry contains 12884 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 QUINOLINATE ACID PHOSPHORIBOSYL TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2095	1301	378	411	5			
1	B	284	Total	C	N	O	S	0	0	0
			2095	1301	378	411	5			
1	C	284	Total	C	N	O	S	0	0	0
			2095	1301	378	411	5			
1	D	284	Total	C	N	O	S	0	0	0
			2095	1301	378	411	5			
1	E	284	Total	C	N	O	S	0	0	0
			2095	1301	378	411	5			
1	F	284	Total	C	N	O	S	0	0	0
			2095	1301	378	411	5			

- 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	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	34	Total O 34 34	0	0
3	B	56	Total O 56 56	0	0
3	C	59	Total O 59 59	0	0
3	D	45	Total O 45 45	0	0
3	E	49	Total O 49 49	0	0
3	F	41	Total O 41 41	0	0

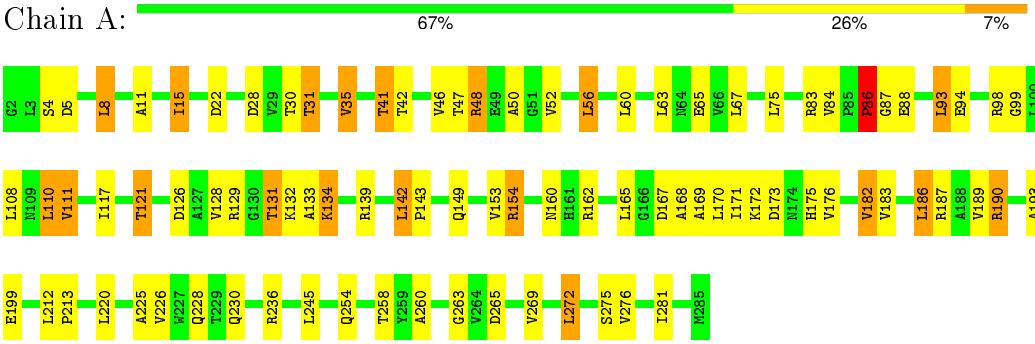
3 Residue-property plots (i)

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.

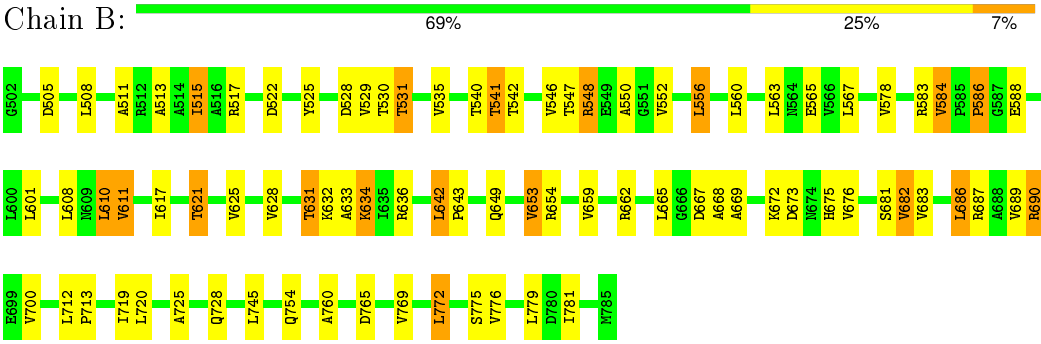
• Molecule 1: QUINOLINATE ACID PHOSPHORIBOSYL TRANSFERASE

Chain A:



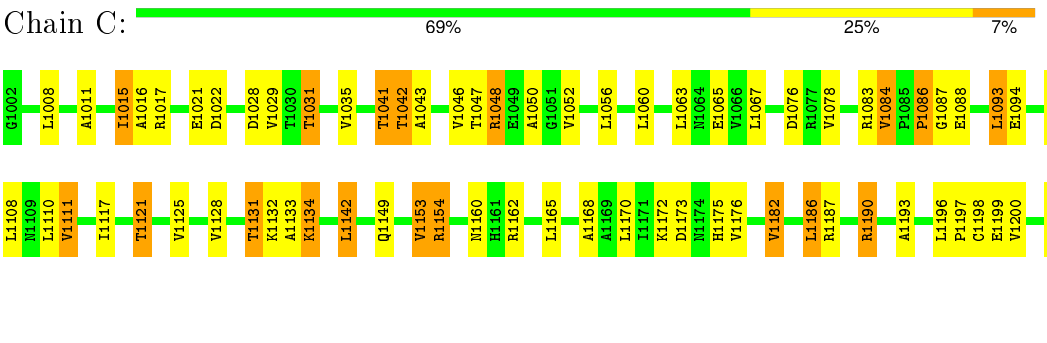
• Molecule 1: QUINOLINATE ACID PHOSPHORIBOSYL TRANSFERASE

Chain B:



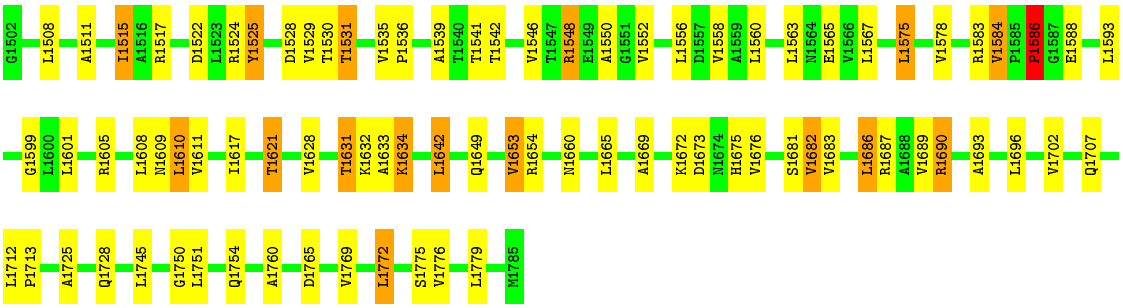
• Molecule 1: QUINOLINATE ACID PHOSPHORIBOSYL TRANSFERASE

Chain C:



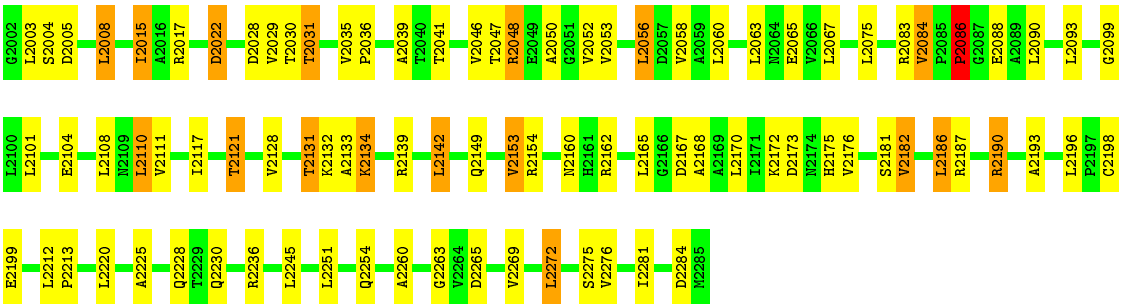
• Molecule 1: QUINOLINATE ACID PHOSPHORIBOSYL TRANSFERASE

Chain D:



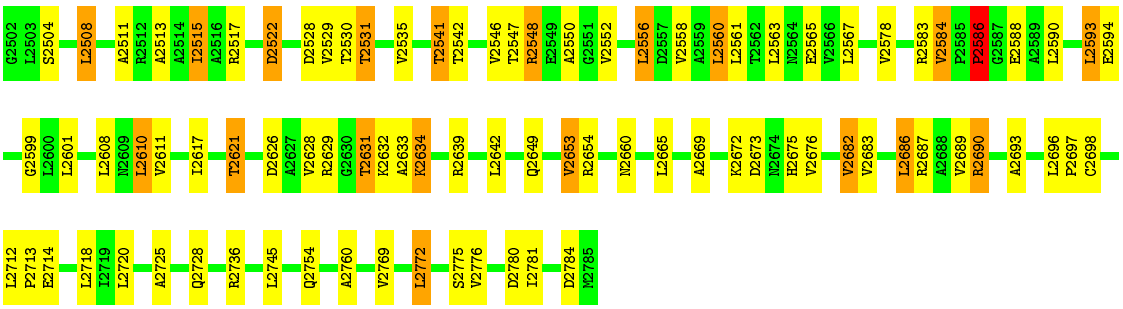
• Molecule 1: QUINOLINATE ACID PHOSPHORIBOSYL TRANSFERASE

Chain E:



• Molecule 1: QUINOLINATE ACID PHOSPHORIBOSYL TRANSFERASE

Chain F:



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 31	Depositor
Cell constants a, b, c, α, β, γ	100.58Å 100.58Å 145.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.40	Depositor
% Data completeness (in resolution range)	94.9 (8.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.176 , 0.242	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12884	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.65	0/2120	0.86	1/2891 (0.0%)
1	B	0.66	0/2120	0.86	1/2891 (0.0%)
1	C	0.67	0/2120	0.87	3/2891 (0.1%)
1	D	0.66	0/2120	0.84	1/2891 (0.0%)
1	E	0.65	0/2120	0.84	0/2891
1	F	0.66	0/2120	0.84	1/2891 (0.0%)
All	All	0.66	0/12720	0.85	7/17346 (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
1	B	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1154	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	B	654	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	C	1154	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	154	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	D	1542	THR	N-CA-C	-5.54	96.03	111.00
1	C	1042	THR	N-CA-C	-5.22	96.91	111.00
1	F	2780	ASP	CB-CG-OD1	5.16	122.94	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	525	TYR	Sidechain
1	D	1525	TYR	Sidechain

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	2095	0	2135	69	0
1	B	2095	0	2135	64	0
1	C	2095	0	2135	65	0
1	D	2095	0	2135	60	0
1	E	2095	0	2135	70	0
1	F	2095	0	2135	70	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	34	0	0	1	0
3	B	56	0	0	2	0
3	C	59	0	0	5	0
3	D	45	0	0	3	0
3	E	49	0	0	1	0
3	F	41	0	0	3	0
All	All	12884	0	12810	356	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 14.

All (356) 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:E:2131:THR:HG21	1:E:2260:ALA:HB1	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:725:ALA:H	1:B:728:GLN:HE21	1.09	0.95
1:A:175:HIS:HE1	1:B:531:THR:HG22	1.31	0.94
1:E:2225:ALA:H	1:E:2228:GLN:HE21	1.18	0.90
1:D:1631:THR:HG21	1:D:1760:ALA:HB1	1.54	0.89
1:D:1515:ILE:HD11	1:D:1565:GLU:HG2	1.54	0.88
1:E:2030:THR:HG22	3:F:3040:HOH:O	1.70	0.88
1:C:1186:LEU:HD22	1:C:1187:ARG:HH21	1.39	0.88
1:A:131:THR:HG21	1:A:260:ALA:HB1	1.58	0.85
1:A:225:ALA:H	1:A:228:GLN:HE21	1.23	0.85
1:A:31:THR:HG22	1:B:675:HIS:HE1	1.42	0.84
1:D:1575:LEU:HD21	3:D:3275:HOH:O	1.77	0.84
1:E:2225:ALA:H	1:E:2228:GLN:NE2	1.75	0.83
1:A:175:HIS:CE1	1:B:531:THR:HG22	2.14	0.83
1:B:631:THR:HG21	1:B:760:ALA:HB1	1.60	0.82
1:F:2725:ALA:H	1:F:2728:GLN:HE21	1.27	0.82
1:A:84:VAL:HG22	1:A:88:GLU:HG2	1.62	0.81
1:B:686:LEU:HD22	1:B:687:ARG:HH21	1.43	0.81
1:E:2134:LYS:HE3	1:E:2265:ASP:O	1.79	0.81
1:C:1175:HIS:HE1	1:D:1531:THR:HG22	1.46	0.81
1:A:186:LEU:HD22	1:A:187:ARG:HH21	1.44	0.81
1:D:1584:VAL:HG22	1:D:1588:GLU:HG2	1.63	0.81
1:E:2275:SER:HA	1:F:2776:VAL:O	1.82	0.80
1:B:725:ALA:H	1:B:728:GLN:NE2	1.80	0.80
1:B:567:LEU:HD21	1:B:599:GLY:HA3	1.63	0.79
1:E:2046:VAL:HG22	1:E:2048:ARG:HH21	1.48	0.78
1:D:1686:LEU:HD22	1:D:1687:ARG:HH21	1.48	0.78
1:D:1725:ALA:H	1:D:1728:GLN:HE21	1.32	0.78
1:A:52:VAL:HG22	1:A:83:ARG:HD2	1.65	0.77
1:C:1046:VAL:HG22	1:C:1048:ARG:HH21	1.49	0.76
1:C:1031:THR:HG22	1:D:1675:HIS:HE1	1.51	0.76
1:B:672:LYS:H	1:B:675:HIS:HD2	1.32	0.75
1:F:2686:LEU:HD22	1:F:2687:ARG:HH21	1.50	0.75
1:C:1225:ALA:H	1:C:1228:GLN:HE21	1.32	0.74
1:D:1567:LEU:HD21	1:D:1599:GLY:HA3	1.68	0.74
1:D:1552:VAL:HG22	1:D:1583:ARG:HD2	1.68	0.74
1:E:2175:HIS:HE1	1:F:2531:THR:HG22	1.54	0.73
1:D:1672:LYS:H	1:D:1675:HIS:HD2	1.37	0.73
1:A:31:THR:HG22	1:B:675:HIS:CE1	2.24	0.73
1:E:2175:HIS:CE1	1:F:2531:THR:HG22	2.24	0.73
1:E:2132:LYS:O	1:E:2134:LYS:HE2	1.89	0.72
1:C:1175:HIS:CE1	1:D:1531:THR:HG22	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1632:LYS:O	1:D:1634:LYS:HE2	1.90	0.72
1:B:632:LYS:O	1:B:634:LYS:HE2	1.89	0.72
1:D:1725:ALA:H	1:D:1728:GLN:NE2	1.87	0.71
1:C:1052:VAL:HG22	1:C:1083:ARG:HD2	1.71	0.71
1:E:2276:VAL:O	1:F:2775:SER:HA	1.90	0.71
1:C:1132:LYS:O	1:C:1134:LYS:HE2	1.91	0.71
1:A:225:ALA:H	1:A:228:GLN:NE2	1.88	0.71
1:A:46:VAL:HG22	1:A:48:ARG:HH21	1.55	0.71
1:B:552:VAL:HG22	1:B:583:ARG:HD2	1.72	0.70
1:F:2584:VAL:HG22	1:F:2588:GLU:HG2	1.73	0.70
1:C:1172:LYS:H	1:C:1175:HIS:HD2	1.39	0.70
1:E:2117:ILE:O	1:E:2121:THR:HG23	1.91	0.70
1:F:2632:LYS:O	1:F:2634:LYS:HE2	1.92	0.69
1:F:2552:VAL:HG22	1:F:2583:ARG:HD2	1.73	0.69
1:F:2672:LYS:H	1:F:2675:HIS:HD2	1.40	0.69
1:A:276:VAL:O	1:B:775:SER:HA	1.93	0.69
1:C:1225:ALA:H	1:C:1228:GLN:NE2	1.91	0.68
1:E:2052:VAL:HG22	1:E:2083:ARG:HD2	1.75	0.68
1:F:2511:ALA:O	1:F:2515:ILE:HG23	1.93	0.68
1:D:1628:VAL:O	1:D:1631:THR:HB	1.94	0.68
1:A:132:LYS:O	1:A:134:LYS:HE2	1.93	0.68
1:F:2631:THR:HG21	1:F:2760:ALA:HB1	1.75	0.68
1:C:1275:SER:HA	1:D:1776:VAL:O	1.93	0.68
1:C:1117:ILE:O	1:C:1121:THR:HG23	1.92	0.68
1:C:1050:ALA:HB2	1:C:1086:PRO:HD3	1.76	0.68
1:B:550:ALA:HB2	1:B:586:PRO:HD3	1.77	0.67
1:C:1276:VAL:O	1:D:1775:SER:HA	1.95	0.67
1:A:172:LYS:H	1:A:175:HIS:HD2	1.43	0.67
1:C:1067:LEU:HD21	1:C:1099:GLY:HA3	1.77	0.67
1:A:41:THR:O	1:A:94:GLU:HA	1.95	0.67
1:C:1154:ARG:HE	1:C:1160:ASN:ND2	1.93	0.66
1:A:128:VAL:O	1:A:131:THR:HB	1.95	0.66
1:C:1131:THR:HG21	1:C:1260:ALA:HB1	1.75	0.66
1:F:2725:ALA:H	1:F:2728:GLN:NE2	1.94	0.66
1:F:2546:VAL:HG22	1:F:2548:ARG:HH21	1.61	0.66
1:B:676:VAL:HG13	1:B:682:VAL:N	2.11	0.65
1:D:1634:LYS:HE3	1:D:1765:ASP:O	1.95	0.65
1:B:662:ARG:HD3	1:B:668:ALA:HB3	1.77	0.65
1:F:2628:VAL:O	1:F:2631:THR:HB	1.96	0.65
1:C:1128:VAL:O	1:C:1131:THR:HB	1.97	0.65
1:A:67:LEU:HD21	1:A:99:GLY:HA3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1511:ALA:O	1:D:1515:ILE:HG23	1.98	0.64
1:E:2031:THR:HG22	1:F:2675:HIS:HE1	1.61	0.64
1:E:2176:VAL:HG13	1:E:2182:VAL:N	2.13	0.64
1:C:1031:THR:HG22	1:D:1675:HIS:CE1	2.32	0.64
1:E:2172:LYS:H	1:E:2175:HIS:HD2	1.46	0.64
1:C:1029:VAL:HG11	1:D:1696:LEU:CD2	2.28	0.64
1:A:176:VAL:HG13	1:A:182:VAL:N	2.13	0.63
1:D:1683:VAL:O	1:D:1687:ARG:HG2	1.99	0.63
1:D:1676:VAL:HG13	1:D:1682:VAL:N	2.14	0.62
1:E:2225:ALA:N	1:E:2228:GLN:HE21	1.93	0.62
1:E:2028:ASP:CG	1:E:2031:THR:HG23	2.20	0.62
1:D:1515:ILE:HD11	1:D:1565:GLU:CG	2.29	0.62
1:A:87:GLY:HA3	1:E:2230:GLN:HB3	1.81	0.62
1:A:162:ARG:HD3	1:A:168:ALA:HB3	1.80	0.62
1:E:2084:VAL:HG22	1:E:2088:GLU:HG2	1.83	0.61
1:B:687:ARG:NH2	1:B:690:ARG:HE	1.99	0.61
1:A:134:LYS:HE3	1:A:265:ASP:O	2.01	0.61
1:F:2617:ILE:O	1:F:2621:THR:HG23	2.01	0.61
1:C:1017:ARG:NH1	1:D:1517:ARG:HD3	2.16	0.61
1:C:1196:LEU:CD2	1:D:1529:VAL:HG11	2.30	0.60
1:D:1546:VAL:HG22	1:D:1548:ARG:HH21	1.66	0.60
1:B:725:ALA:N	1:B:728:GLN:HE21	1.91	0.60
1:E:2128:VAL:O	1:E:2131:THR:HB	2.01	0.60
1:A:172:LYS:O	1:A:176:VAL:HG23	2.01	0.60
1:F:2676:VAL:HG13	1:F:2682:VAL:N	2.17	0.60
1:E:2017:ARG:HD3	1:F:2517:ARG:NH1	2.17	0.59
1:F:2515:ILE:HD11	1:F:2565:GLU:HG2	1.84	0.59
1:F:2769:VAL:HB	1:F:2772:LEU:HD22	1.85	0.59
1:B:631:THR:CG2	1:B:633:ALA:H	2.14	0.59
1:F:2683:VAL:HG12	1:F:2714:GLU:HG3	1.85	0.59
1:C:1015:ILE:HD11	1:C:1065:GLU:HG2	1.84	0.59
1:B:546:VAL:HG22	1:B:548:ARG:HH21	1.66	0.58
1:A:117:ILE:O	1:A:121:THR:HG23	2.02	0.58
1:A:131:THR:HG23	1:A:133:ALA:H	1.67	0.58
1:E:2196:LEU:CD2	1:F:2529:VAL:HG11	2.34	0.58
1:A:275:SER:HA	1:B:776:VAL:O	2.03	0.58
1:E:2186:LEU:HD22	1:E:2187:ARG:HH21	1.68	0.58
1:E:2162:ARG:HD3	1:E:2168:ALA:HB3	1.85	0.58
1:C:1134:LYS:HE3	1:C:1265:ASP:O	2.04	0.57
1:E:2029:VAL:HG11	1:F:2696:LEU:CD2	2.34	0.57
1:E:2029:VAL:HG21	1:F:2693:ALA:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1642:LEU:H	1:D:1649:GLN:HE22	1.52	0.57
1:C:1142:LEU:H	1:C:1149:GLN:HE22	1.49	0.57
1:B:769:VAL:HB	1:B:772:LEU:HD22	1.85	0.57
1:E:2121:THR:HG21	1:E:2153:VAL:HA	1.85	0.57
1:A:131:THR:CG2	1:A:133:ALA:H	2.17	0.57
1:E:2131:THR:CG2	1:E:2133:ALA:H	2.18	0.57
1:C:1154:ARG:HE	1:C:1160:ASN:HD21	1.50	0.57
1:A:50:ALA:HB2	1:A:86:PRO:HD3	1.86	0.57
1:B:683:VAL:O	1:B:687:ARG:HG2	2.05	0.56
1:C:1011:ALA:O	1:C:1015:ILE:HG23	2.05	0.56
1:F:2654:ARG:HE	1:F:2660:ASN:ND2	2.03	0.56
1:D:1687:ARG:NH2	1:D:1690:ARG:HE	2.03	0.56
1:E:2083:ARG:HB3	3:E:3090:HOH:O	2.05	0.56
1:B:584:VAL:HG22	1:B:588:GLU:HG2	1.87	0.56
1:A:196:LEU:HD23	1:B:529:VAL:HG11	1.87	0.56
1:C:1029:VAL:HG21	1:D:1693:ALA:HB2	1.88	0.56
1:B:662:ARG:HD2	1:B:667:ASP:HB3	1.87	0.56
1:E:2015:ILE:HD11	1:E:2065:GLU:HG2	1.86	0.56
1:D:1769:VAL:HB	1:D:1772:LEU:HD22	1.88	0.56
1:D:1524:ARG:HD3	3:D:3215:HOH:O	2.05	0.55
1:C:1239:ARG:NH1	3:C:3266:HOH:O	2.38	0.55
1:E:2193:ALA:HB2	1:F:2529:VAL:HG21	1.88	0.55
1:D:1621:THR:HG21	1:D:1653:VAL:HA	1.89	0.55
1:D:1528:ASP:CG	1:D:1531:THR:HG23	2.26	0.55
1:A:15:ILE:HD11	1:A:65:GLU:HG2	1.89	0.55
1:A:154:ARG:HE	1:A:160:ASN:ND2	2.04	0.55
1:B:672:LYS:H	1:B:675:HIS:CD2	2.20	0.54
1:A:187:ARG:NH2	1:A:190:ARG:HE	2.05	0.54
1:E:2121:THR:HG22	1:E:2272:LEU:HG	1.90	0.54
1:E:2017:ARG:NH1	1:F:2517:ARG:HD3	2.21	0.54
1:A:111:VAL:HG23	1:A:281:ILE:HD12	1.89	0.54
1:E:2047:THR:O	1:E:2086:PRO:O	2.26	0.54
1:A:193:ALA:HB2	1:B:529:VAL:HG21	1.88	0.54
1:A:11:ALA:O	1:A:15:ILE:HG23	2.06	0.54
1:B:628:VAL:O	1:B:631:THR:HB	2.07	0.54
1:E:2154:ARG:HE	1:E:2160:ASN:ND2	2.06	0.53
1:E:2058:VAL:HG11	1:E:2110:LEU:HG	1.90	0.53
1:B:541:THR:O	1:B:594:GLU:HA	2.09	0.53
1:D:1550:ALA:HB2	1:D:1586:PRO:HD3	1.90	0.53
1:E:2031:THR:HG22	1:F:2675:HIS:CE1	2.43	0.53
1:C:1176:VAL:HG13	1:C:1182:VAL:N	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1084:VAL:HG22	1:C:1088:GLU:HG2	1.89	0.53
1:B:513:ALA:O	1:B:517:ARG:HG3	2.09	0.53
1:E:2131:THR:HG23	1:E:2133:ALA:H	1.72	0.53
1:B:617:ILE:O	1:B:621:THR:CG2	2.57	0.53
1:A:121:THR:HG22	1:A:272:LEU:HG	1.91	0.53
1:B:617:ILE:O	1:B:621:THR:HG23	2.09	0.53
1:F:2621:THR:HG21	1:F:2653:VAL:HA	1.90	0.53
1:A:196:LEU:CD2	1:B:529:VAL:HG11	2.38	0.53
1:A:139:ARG:NH2	3:A:3130:HOH:O	2.42	0.53
1:B:676:VAL:HG22	1:B:682:VAL:HA	1.90	0.53
1:F:2672:LYS:H	1:F:2675:HIS:CD2	2.25	0.52
1:F:2683:VAL:O	1:F:2687:ARG:HG2	2.10	0.52
1:F:2542:THR:HA	1:F:2593:LEU:O	2.09	0.52
1:C:1047:THR:O	1:C:1086:PRO:O	2.28	0.52
1:E:2047:THR:HG23	1:E:2090:LEU:HD11	1.91	0.52
1:E:2236:ARG:C	1:E:2236:ARG:HD2	2.30	0.51
1:E:2142:LEU:H	1:E:2149:GLN:HE22	1.58	0.51
1:B:687:ARG:HH22	1:B:690:ARG:HE	1.56	0.51
1:A:183:VAL:O	1:A:187:ARG:HG2	2.10	0.51
1:F:2631:THR:HG23	1:F:2633:ALA:H	1.74	0.51
1:C:1193:ALA:HB2	1:D:1529:VAL:HG21	1.93	0.51
1:A:42:THR:HA	1:A:93:LEU:O	2.10	0.51
1:C:1028:ASP:CG	1:C:1031:THR:HG23	2.31	0.50
1:F:2687:ARG:NH2	1:F:2690:ARG:HE	2.09	0.50
1:E:2187:ARG:NH2	1:E:2190:ARG:HE	2.09	0.50
1:F:2547:THR:HG22	1:F:2781:ILE:HG12	1.92	0.50
1:A:126:ASP:O	1:A:129:ARG:HG2	2.12	0.50
1:E:2196:LEU:HD23	1:F:2529:VAL:HG11	1.93	0.50
1:D:1654:ARG:HE	1:D:1660:ASN:ND2	2.09	0.50
1:C:1117:ILE:O	1:C:1121:THR:CG2	2.58	0.50
1:A:28:ASP:CG	1:A:31:THR:HG23	2.31	0.50
1:B:611:VAL:HG23	1:B:781:ILE:HD12	1.93	0.50
1:B:634:LYS:HE3	1:B:765:ASP:O	2.11	0.49
1:E:2004:SER:O	1:E:2008:LEU:HB2	2.12	0.49
1:A:172:LYS:H	1:A:175:HIS:CD2	2.28	0.49
1:E:2067:LEU:HD21	1:E:2099:GLY:HA3	1.93	0.49
1:F:2626:ASP:O	1:F:2629:ARG:HG2	2.12	0.49
1:C:1225:ALA:N	1:C:1228:GLN:HE21	2.07	0.49
1:C:1131:THR:CG2	1:C:1133:ALA:H	2.26	0.49
1:A:47:THR:O	1:A:86:PRO:O	2.31	0.49
1:B:642:LEU:H	1:B:649:GLN:HE22	1.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:N	1:A:213:PRO:HD2	2.28	0.49
1:D:1672:LYS:H	1:D:1675:HIS:CD2	2.23	0.49
1:F:2515:ILE:HD11	1:F:2565:GLU:CB	2.42	0.48
1:B:712:LEU:N	1:B:713:PRO:HD2	2.28	0.48
1:B:547:THR:O	1:B:586:PRO:O	2.31	0.48
1:C:1131:THR:HG23	1:C:1133:ALA:H	1.79	0.48
1:E:2154:ARG:HE	1:E:2160:ASN:HD21	1.61	0.48
1:B:528:ASP:CG	1:B:531:THR:HG23	2.34	0.48
1:F:2631:THR:CG2	1:F:2633:ALA:H	2.25	0.48
1:B:631:THR:HG23	1:B:633:ALA:H	1.77	0.48
1:A:143:PRO:HG3	1:B:610:LEU:HD13	1.95	0.48
1:C:1170:LEU:HD23	1:C:1199:GLU:HB2	1.95	0.48
1:B:631:THR:HG22	1:B:633:ALA:H	1.79	0.48
1:B:540:THR:HG22	3:B:3127:HOH:O	2.13	0.48
1:E:2117:ILE:O	1:E:2121:THR:CG2	2.61	0.47
1:D:1725:ALA:N	1:D:1728:GLN:HE21	2.06	0.47
1:E:2170:LEU:HA	1:E:2199:GLU:O	2.14	0.47
1:E:2036:PRO:HG2	1:E:2039:ALA:HB2	1.96	0.47
1:E:2139:ARG:NH1	1:F:2522:ASP:OD2	2.48	0.47
1:F:2586:PRO:HB2	3:F:3114:HOH:O	2.14	0.47
1:E:2176:VAL:HG22	1:E:2182:VAL:HA	1.96	0.47
1:E:2111:VAL:HG23	1:E:2281:ILE:HD12	1.97	0.47
1:D:1669:ALA:HB1	1:D:1689:VAL:HG11	1.96	0.47
1:C:1172:LYS:H	1:C:1175:HIS:CD2	2.25	0.47
1:A:121:THR:HG21	1:A:153:VAL:HA	1.96	0.47
1:D:1617:ILE:O	1:D:1621:THR:CG2	2.63	0.47
1:C:1162:ARG:HD3	1:C:1168:ALA:HB3	1.96	0.47
1:A:226:VAL:HG11	1:A:258:THR:HG22	1.96	0.47
1:F:2617:ILE:O	1:F:2621:THR:CG2	2.62	0.47
1:A:269:VAL:HB	1:A:272:LEU:HD22	1.96	0.47
1:F:2567:LEU:HD21	1:F:2599:GLY:HA3	1.97	0.47
1:E:2053:VAL:HG21	1:E:2056:LEU:HD22	1.97	0.47
1:C:1226:VAL:HG11	1:C:1258:THR:HG22	1.97	0.47
1:C:1043:ALA:HB2	1:C:1285:MET:HG2	1.97	0.47
1:E:2132:LYS:HE2	1:E:2263:GLY:O	2.14	0.46
1:C:1041:THR:O	1:C:1094:GLU:HA	2.15	0.46
1:A:132:LYS:HE2	1:A:263:GLY:O	2.14	0.46
1:C:1029:VAL:HG11	1:D:1696:LEU:HD23	1.97	0.46
1:C:1142:LEU:H	1:C:1149:GLN:NE2	2.12	0.46
1:F:2654:ARG:HE	1:F:2660:ASN:HD21	1.61	0.46
1:F:2712:LEU:N	1:F:2713:PRO:HD2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:2550:ALA:HB2	1:F:2586:PRO:HD3	1.98	0.46
1:D:1676:VAL:HG22	1:D:1682:VAL:HA	1.97	0.46
1:E:2212:LEU:N	1:E:2213:PRO:HD2	2.31	0.46
1:F:2687:ARG:HH22	1:F:2690:ARG:HE	1.62	0.46
1:C:1190:ARG:NH2	1:C:1214:GLU:O	2.49	0.46
1:F:2548:ARG:NH2	1:F:2784:ASP:OD2	2.49	0.46
1:A:187:ARG:HH22	1:A:190:ARG:HE	1.63	0.46
1:D:1617:ILE:O	1:D:1621:THR:HG23	2.16	0.46
1:D:1642:LEU:H	1:D:1649:GLN:NE2	2.13	0.46
1:F:2541:THR:O	1:F:2594:GLU:HA	2.16	0.46
1:E:2134:LYS:CE	1:E:2265:ASP:O	2.59	0.45
1:B:515:ILE:HD11	1:B:565:GLU:HG2	1.98	0.45
1:B:642:LEU:H	1:B:649:GLN:NE2	2.14	0.45
1:F:2513:ALA:O	1:F:2517:ARG:HG3	2.16	0.45
1:D:1631:THR:CG2	1:D:1633:ALA:H	2.28	0.45
1:A:56:LEU:HD12	1:A:56:LEU:HA	1.86	0.45
1:A:176:VAL:HG22	1:A:182:VAL:HA	1.99	0.45
1:C:1047:THR:HG22	1:C:1281:ILE:HG12	1.99	0.45
1:F:2649:GLN:O	1:F:2653:VAL:HG13	2.16	0.45
1:F:2669:ALA:HA	3:F:3040:HOH:O	2.17	0.45
1:A:171:ILE:HD13	1:A:186:LEU:HA	1.98	0.45
1:B:700:VAL:O	1:B:719:ILE:HA	2.17	0.45
1:A:162:ARG:HD2	1:A:167:ASP:HB3	1.98	0.45
1:C:1200:VAL:O	1:C:1219:ILE:HA	2.16	0.45
1:A:4:SER:O	1:A:8:LEU:HB2	2.17	0.44
1:D:1687:ARG:HH22	1:D:1690:ARG:HE	1.63	0.44
1:D:1536:PRO:HG2	1:D:1539:ALA:HB2	1.98	0.44
1:A:225:ALA:N	1:A:228:GLN:HE21	2.02	0.44
1:D:1649:GLN:O	1:D:1653:VAL:HG13	2.17	0.44
1:B:696:LEU:HA	1:B:697:PRO:HD3	1.92	0.44
1:B:669:ALA:HB1	1:B:689:VAL:HG11	1.99	0.44
1:F:2696:LEU:HA	1:F:2697:PRO:HD3	1.88	0.44
1:E:2172:LYS:O	1:E:2176:VAL:HG23	2.17	0.44
1:B:547:THR:HG22	1:B:781:ILE:HG12	1.99	0.44
1:B:511:ALA:O	1:B:515:ILE:HG23	2.17	0.44
1:B:621:THR:HG21	1:B:653:VAL:HA	2.00	0.44
1:C:1121:THR:HG22	1:C:1272:LEU:HG	2.00	0.44
1:F:2508:LEU:HD11	1:F:2561:LEU:HD21	2.00	0.44
1:B:676:VAL:HG13	1:B:681:SER:C	2.38	0.44
1:C:1172:LYS:HE3	1:C:1172:LYS:HB2	1.68	0.43
1:E:2048:ARG:HH22	1:E:2284:ASP:CG	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ILE:HD12	1:A:15:ILE:C	2.37	0.43
1:A:35:VAL:O	1:A:98:ARG:NE	2.48	0.43
1:A:142:LEU:H	1:A:149:GLN:HE22	1.66	0.43
1:D:1515:ILE:HD11	1:D:1565:GLU:CB	2.48	0.43
1:A:230:GLN:HB3	1:C:1087:GLY:HA3	1.99	0.43
1:F:2683:VAL:HG12	1:F:2714:GLU:CG	2.48	0.43
1:F:2686:LEU:HD13	1:F:2714:GLU:HB3	2.01	0.43
1:C:1121:THR:HG21	1:C:1153:VAL:HA	2.00	0.43
1:C:1212:LEU:N	1:C:1213:PRO:HD2	2.33	0.43
1:C:1042:THR:HA	1:C:1093:LEU:O	2.18	0.43
1:B:779:LEU:HA	1:B:779:LEU:HD12	1.91	0.43
1:A:170:LEU:HA	1:A:199:GLU:O	2.17	0.43
1:C:1198:CYS:O	1:C:1217:GLU:HB2	2.18	0.43
1:D:1558:VAL:HG11	1:D:1610:LEU:HG	2.01	0.43
1:A:169:ALA:HB1	1:A:189:VAL:HG11	2.01	0.43
1:F:2515:ILE:HD11	1:F:2565:GLU:CG	2.48	0.43
1:A:193:ALA:CB	1:B:529:VAL:HG21	2.48	0.43
1:F:2504:SER:O	1:F:2508:LEU:HB2	2.19	0.43
1:F:2736:ARG:C	1:F:2736:ARG:HD2	2.39	0.43
1:A:117:ILE:O	1:A:121:THR:CG2	2.65	0.42
1:F:2558:VAL:HG11	1:F:2610:LEU:HG	2.01	0.42
1:F:2556:LEU:HD12	1:F:2556:LEU:HA	1.83	0.42
1:C:1134:LYS:HG2	3:C:3220:HOH:O	2.19	0.42
1:C:1269:VAL:HB	1:C:1272:LEU:HD22	2.00	0.42
1:A:110:LEU:HD13	1:B:643:PRO:HG3	2.00	0.42
1:D:1750:GLY:N	3:D:3183:HOH:O	2.50	0.42
1:D:1712:LEU:N	1:D:1713:PRO:HD2	2.34	0.42
1:B:687:ARG:NH2	1:B:690:ARG:NE	2.67	0.42
1:B:621:THR:O	1:B:625:VAL:HG23	2.20	0.42
1:C:1016:ALA:HB2	3:C:3260:HOH:O	2.20	0.42
1:E:2050:ALA:HB2	1:E:2086:PRO:HD3	2.02	0.42
1:A:142:LEU:H	1:A:149:GLN:NE2	2.18	0.42
1:E:2176:VAL:HG13	1:E:2181:SER:C	2.41	0.42
1:E:2003:LEU:HB2	1:E:2008:LEU:CD2	2.50	0.42
1:B:542:THR:HA	1:B:593:LEU:O	2.19	0.41
1:E:2269:VAL:HB	1:E:2272:LEU:HD22	2.02	0.41
1:A:236:ARG:C	1:A:236:ARG:HD2	2.40	0.41
1:F:2528:ASP:CG	1:F:2531:THR:HG23	2.41	0.41
1:A:105:ARG:HG3	3:B:3157:HOH:O	2.19	0.41
1:F:2669:ALA:HB1	1:F:2689:VAL:HG11	2.03	0.41
1:E:2048:ARG:NH2	1:E:2284:ASP:OD2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:696:LEU:HA	1:B:696:LEU:HD12	1.93	0.41
1:F:2556:LEU:O	1:F:2560:LEU:HD22	2.20	0.41
1:E:2075:LEU:N	1:E:2075:LEU:CD1	2.83	0.41
1:D:1525:TYR:CD1	1:D:1525:TYR:N	2.88	0.41
1:D:1605:ARG:HD3	1:D:1609:ASN:OD1	2.19	0.41
1:D:1676:VAL:HG13	1:D:1681:SER:C	2.41	0.41
1:E:2029:VAL:HG11	1:F:2696:LEU:HD21	2.01	0.41
1:C:1076:ASP:HB3	3:C:3253:HOH:O	2.21	0.41
1:C:1121:THR:O	1:C:1125:VAL:HG23	2.21	0.41
1:C:1111:VAL:HG23	1:C:1281:ILE:HD12	2.03	0.41
1:B:556:LEU:HA	1:B:556:LEU:HD12	1.94	0.41
1:F:2672:LYS:HE3	1:F:2672:LYS:HB2	1.82	0.40
1:C:1154:ARG:HG2	3:C:3218:HOH:O	2.21	0.40
1:F:2676:VAL:HG22	1:F:2682:VAL:HA	2.02	0.40
1:B:636:ARG:CD	1:B:659:VAL:HG22	2.51	0.40
1:D:1515:ILE:HD12	1:D:1515:ILE:C	2.42	0.40
1:E:2172:LYS:H	1:E:2175:HIS:CD2	2.31	0.40
1:D:1654:ARG:HE	1:D:1660:ASN:HD21	1.68	0.40
1:C:1196:LEU:HA	1:C:1197:PRO:HD3	1.98	0.40
1:A:154:ARG:HE	1:A:160:ASN:HD21	1.69	0.40
1:D:1702:VAL:HA	1:D:1707:GLN:OE1	2.21	0.40
1:E:2172:LYS:HE3	1:E:2172:LYS:HB2	1.80	0.40
1:C:1017:ARG:O	1:C:1021:GLU:HG3	2.20	0.40
1:E:2022:ASP:OD2	1:F:2639:ARG:NH1	2.55	0.40
1:E:2162:ARG:HD2	1:E:2167:ASP:HB3	2.03	0.40
1:F:2547:THR:HG23	1:F:2590:LEU:HD11	2.02	0.40
1:D:1779:LEU:HA	1:D:1779:LEU:HD12	1.89	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	282/284 (99%)	274 (97%)	7 (2%)	1 (0%)	39	56
1	B	282/284 (99%)	276 (98%)	6 (2%)	0	100	100
1	C	282/284 (99%)	276 (98%)	6 (2%)	0	100	100
1	D	282/284 (99%)	277 (98%)	4 (1%)	1 (0%)	39	56
1	E	282/284 (99%)	275 (98%)	5 (2%)	2 (1%)	26	38
1	F	282/284 (99%)	277 (98%)	4 (1%)	1 (0%)	39	56
All	All	1692/1704 (99%)	1655 (98%)	32 (2%)	5 (0%)	46	63

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	2104	GLU
1	F	2586	PRO
1	D	1586	PRO
1	A	86	PRO
1	E	2086	PRO

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	216/216 (100%)	183 (85%)	33 (15%)	3	4
1	B	216/216 (100%)	181 (84%)	35 (16%)	3	3
1	C	216/216 (100%)	185 (86%)	31 (14%)	4	4
1	D	216/216 (100%)	182 (84%)	34 (16%)	3	3
1	E	216/216 (100%)	183 (85%)	33 (15%)	3	4
1	F	216/216 (100%)	181 (84%)	35 (16%)	3	3
All	All	1296/1296 (100%)	1095 (84%)	201 (16%)	3	4

All (201) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASP
1	A	8	LEU
1	A	15	ILE
1	A	22	ASP
1	A	30	THR
1	A	31	THR
1	A	35	VAL
1	A	41	THR
1	A	48	ARG
1	A	56	LEU
1	A	60	LEU
1	A	63	LEU
1	A	75	LEU
1	A	86	PRO
1	A	93	LEU
1	A	101	LEU
1	A	108	LEU
1	A	110	LEU
1	A	111	VAL
1	A	121	THR
1	A	131	THR
1	A	134	LYS
1	A	142	LEU
1	A	165	LEU
1	A	173	ASP
1	A	182	VAL
1	A	186	LEU
1	A	190	ARG
1	A	198	CYS
1	A	220	LEU
1	A	245	LEU
1	A	254	GLN
1	A	272	LEU
1	B	505	ASP
1	B	508	LEU
1	B	515	ILE
1	B	522	ASP
1	B	530	THR
1	B	531	THR
1	B	535	VAL
1	B	541	THR
1	B	548	ARG
1	B	556	LEU

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Mol	Chain	Res	Type
1	B	560	LEU
1	B	563	LEU
1	B	578	VAL
1	B	584	VAL
1	B	586	PRO
1	B	593	LEU
1	B	601	LEU
1	B	608	LEU
1	B	610	LEU
1	B	611	VAL
1	B	621	THR
1	B	631	THR
1	B	634	LYS
1	B	642	LEU
1	B	653	VAL
1	B	665	LEU
1	B	673	ASP
1	B	682	VAL
1	B	686	LEU
1	B	690	ARG
1	B	698	CYS
1	B	720	LEU
1	B	745	LEU
1	B	754	GLN
1	B	772	LEU
1	C	1008	LEU
1	C	1015	ILE
1	C	1022	ASP
1	C	1031	THR
1	C	1035	VAL
1	C	1041	THR
1	C	1048	ARG
1	C	1056	LEU
1	C	1060	LEU
1	C	1063	LEU
1	C	1078	VAL
1	C	1084	VAL
1	C	1086	PRO
1	C	1093	LEU
1	C	1101	LEU
1	C	1108	LEU
1	C	1110	LEU

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Mol	Chain	Res	Type
1	C	1111	VAL
1	C	1121	THR
1	C	1131	THR
1	C	1134	LYS
1	C	1142	LEU
1	C	1153	VAL
1	C	1165	LEU
1	C	1173	ASP
1	C	1182	VAL
1	C	1186	LEU
1	C	1190	ARG
1	C	1245	LEU
1	C	1254	GLN
1	C	1272	LEU
1	D	1508	LEU
1	D	1515	ILE
1	D	1522	ASP
1	D	1530	THR
1	D	1531	THR
1	D	1535	VAL
1	D	1541	THR
1	D	1548	ARG
1	D	1556	LEU
1	D	1560	LEU
1	D	1563	LEU
1	D	1575	LEU
1	D	1578	VAL
1	D	1584	VAL
1	D	1586	PRO
1	D	1593	LEU
1	D	1601	LEU
1	D	1608	LEU
1	D	1610	LEU
1	D	1611	VAL
1	D	1621	THR
1	D	1631	THR
1	D	1634	LYS
1	D	1642	LEU
1	D	1653	VAL
1	D	1665	LEU
1	D	1673	ASP
1	D	1682	VAL

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Mol	Chain	Res	Type
1	D	1686	LEU
1	D	1690	ARG
1	D	1745	LEU
1	D	1751	LEU
1	D	1754	GLN
1	D	1772	LEU
1	E	2005	ASP
1	E	2008	LEU
1	E	2015	ILE
1	E	2022	ASP
1	E	2031	THR
1	E	2035	VAL
1	E	2041	THR
1	E	2048	ARG
1	E	2056	LEU
1	E	2060	LEU
1	E	2063	LEU
1	E	2084	VAL
1	E	2086	PRO
1	E	2093	LEU
1	E	2101	LEU
1	E	2108	LEU
1	E	2110	LEU
1	E	2121	THR
1	E	2131	THR
1	E	2134	LYS
1	E	2142	LEU
1	E	2153	VAL
1	E	2165	LEU
1	E	2173	ASP
1	E	2182	VAL
1	E	2186	LEU
1	E	2190	ARG
1	E	2198	CYS
1	E	2220	LEU
1	E	2245	LEU
1	E	2251	LEU
1	E	2254	GLN
1	E	2272	LEU
1	F	2508	LEU
1	F	2515	ILE
1	F	2522	ASP

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Mol	Chain	Res	Type
1	F	2530	THR
1	F	2531	THR
1	F	2535	VAL
1	F	2541	THR
1	F	2548	ARG
1	F	2556	LEU
1	F	2560	LEU
1	F	2563	LEU
1	F	2578	VAL
1	F	2584	VAL
1	F	2586	PRO
1	F	2593	LEU
1	F	2601	LEU
1	F	2608	LEU
1	F	2610	LEU
1	F	2611	VAL
1	F	2621	THR
1	F	2631	THR
1	F	2634	LYS
1	F	2642	LEU
1	F	2653	VAL
1	F	2665	LEU
1	F	2673	ASP
1	F	2682	VAL
1	F	2686	LEU
1	F	2690	ARG
1	F	2698	CYS
1	F	2718	LEU
1	F	2720	LEU
1	F	2745	LEU
1	F	2754	GLN
1	F	2772	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	GLN
1	A	160	ASN
1	A	174	ASN
1	A	175	HIS
1	A	228	GLN
1	B	649	GLN

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Mol	Chain	Res	Type
1	B	660	ASN
1	B	675	HIS
1	B	728	GLN
1	C	1149	GLN
1	C	1160	ASN
1	C	1174	ASN
1	C	1175	HIS
1	C	1228	GLN
1	C	1234	GLN
1	D	1649	GLN
1	D	1660	ASN
1	D	1674	ASN
1	D	1675	HIS
1	D	1728	GLN
1	E	2149	GLN
1	E	2160	ASN
1	E	2174	ASN
1	E	2175	HIS
1	E	2228	GLN
1	F	2649	GLN
1	F	2660	ASN
1	F	2674	ASN
1	F	2675	HIS
1	F	2728	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

6 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	2985	-	4,4,4	1.47	1 (25%)	6,6,6	0.34	0
2	SO4	B	2986	-	4,4,4	1.78	2 (50%)	6,6,6	0.47	0
2	SO4	C	2987	-	4,4,4	2.02	2 (50%)	6,6,6	0.54	0
2	SO4	D	2990	-	4,4,4	1.65	1 (25%)	6,6,6	0.19	0
2	SO4	E	2989	-	4,4,4	1.66	1 (25%)	6,6,6	0.27	0
2	SO4	F	2988	-	4,4,4	1.38	0	6,6,6	0.28	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	2985	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2986	-	-	0/0/0/0	0/0/0/0
2	SO4	C	2987	-	-	0/0/0/0	0/0/0/0
2	SO4	D	2990	-	-	0/0/0/0	0/0/0/0
2	SO4	E	2989	-	-	0/0/0/0	0/0/0/0
2	SO4	F	2988	-	-	0/0/0/0	0/0/0/0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2985	SO4	O3-S	2.01	1.54	1.47
2	C	2987	SO4	O2-S	2.11	1.54	1.47
2	B	2986	SO4	O4-S	2.12	1.55	1.47
2	B	2986	SO4	O3-S	2.21	1.55	1.47
2	E	2989	SO4	O3-S	2.22	1.55	1.47
2	D	2990	SO4	O3-S	2.55	1.56	1.47
2	C	2987	SO4	O3-S	3.00	1.58	1.47

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

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

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

6.3 Carbohydrates

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

6.4 Ligands

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

6.5 Other polymers

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