



Full wwPDB X-ray Structure Validation Report i

Feb 26, 2014 – 04:28 PM GMT

PDB ID : 1QPQ
Title : Structure of Quinolinic Acid Phosphoribosyltransferase from Mycobacterium
Tuberculosis: A Potential TB Drug Target
Authors : Sharma, V.; Grubmeyer, C.; Sacchettini, J.C.; TB Structural Genomics Con-
sortium (TBSGC)
Deposited on : 1998-11-20
Resolution : 2.45 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

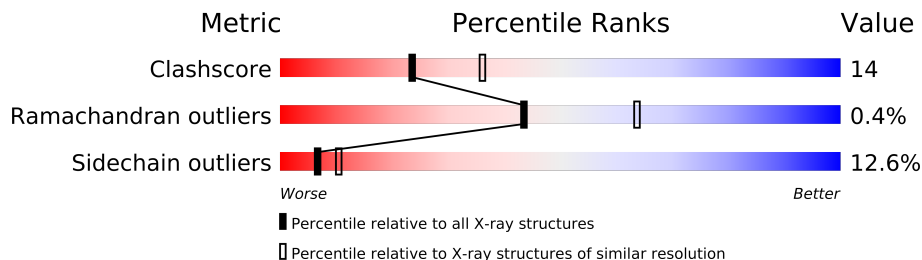
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	21963
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.45 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	79885	4471 (2.50-2.42)
Ramachandran outliers	78287	4383 (2.50-2.42)
Sidechain outliers	78261	4385 (2.50-2.42)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	284	
1	B	284	
1	C	284	
1	D	284	
1	E	284	
1	F	284	

2 Entry composition

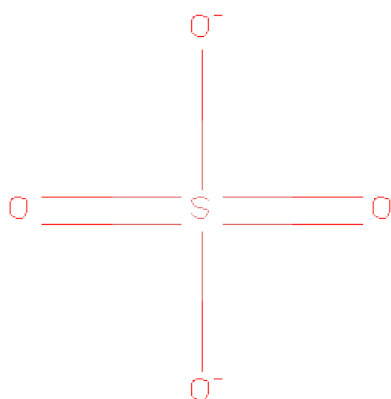
There are 4 unique types of molecules in this entry. The entry contains 12938 atoms, of which 0 are hydrogen and 0 are deuterium.

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 PHOSPHORIBOSYLTRANSFERASE.

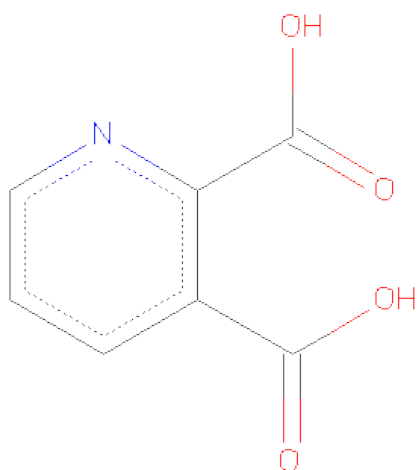
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	0	0
			2095	1301	378	411	5			
1	B	284	Total	C	N	O	S	0	0	0
			2095	1301	378	411	5			
1	C	284	Total	C	N	O	S	0	0	0
			2095	1301	378	411	5			
1	D	284	Total	C	N	O	S	0	0	0
			2095	1301	378	411	5			
1	E	284	Total	C	N	O	S	0	0	0
			2095	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: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is QUINOLINIC ACID (three-letter code: NTM) (formula: $C_7H_5NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	7	1	4		
3	B	1	Total	C	N	O	0	0
			12	7	1	4		
3	C	1	Total	C	N	O	0	0
			12	7	1	4		
3	D	1	Total	C	N	O	0	0
			12	7	1	4		
3	E	1	Total	C	N	O	0	0
			12	7	1	4		
3	F	1	Total	C	N	O	0	0
			12	7	1	4		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	36	Total 36	O 36	0	0
4	B	47	Total 47	O 47	0	0
4	C	60	Total 60	O 60	0	0
4	D	43	Total 43	O 43	0	0
4	E	47	Total 47	O 47	0	0
4	F	33	Total 33	O 33	0	0

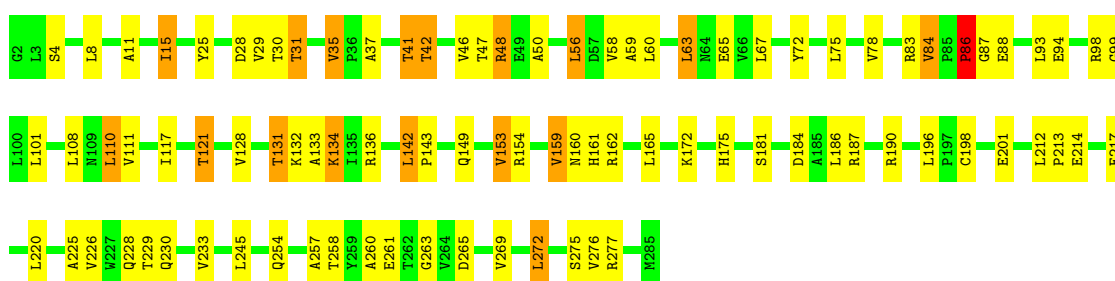
3 Residue-property plots

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.

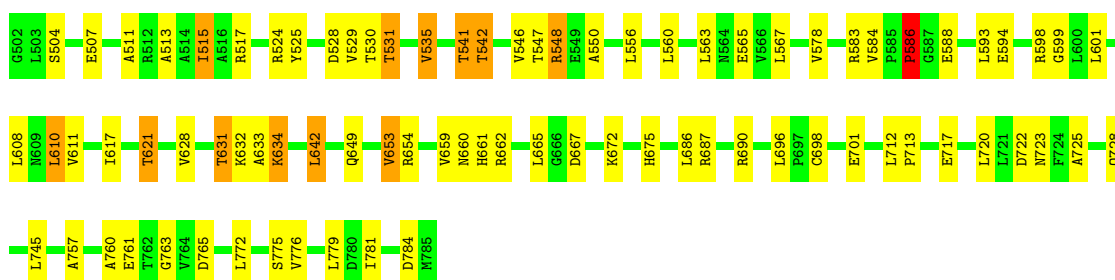
• Molecule 1: QUINOLINATE PHOSPHORIBOSYLTRANSFERASE

Chain A:



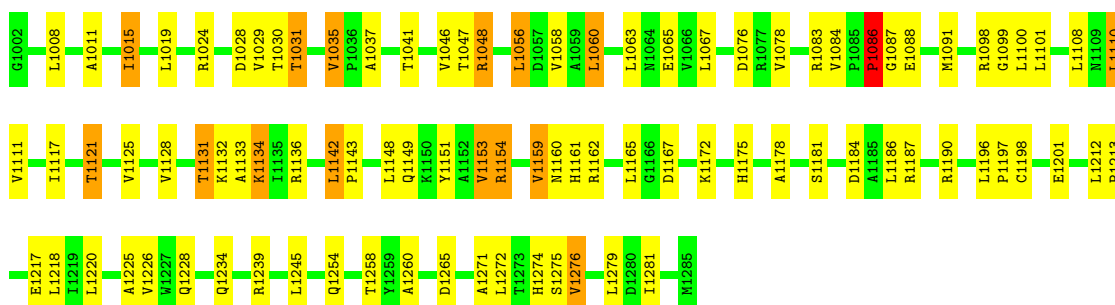
• Molecule 1: QUINOLINATE PHOSPHORIBOSYLTRANSFERASE

Chain B:



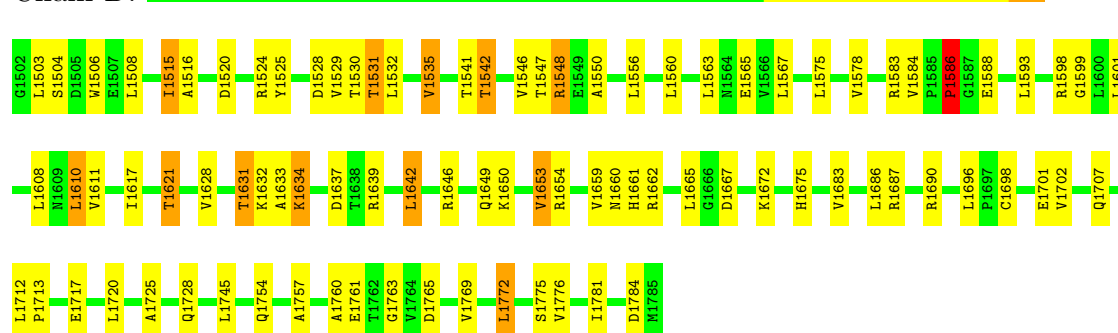
• Molecule 1: QUINOLINATE PHOSPHORIBOSYLTRANSFERASE

Chain C:



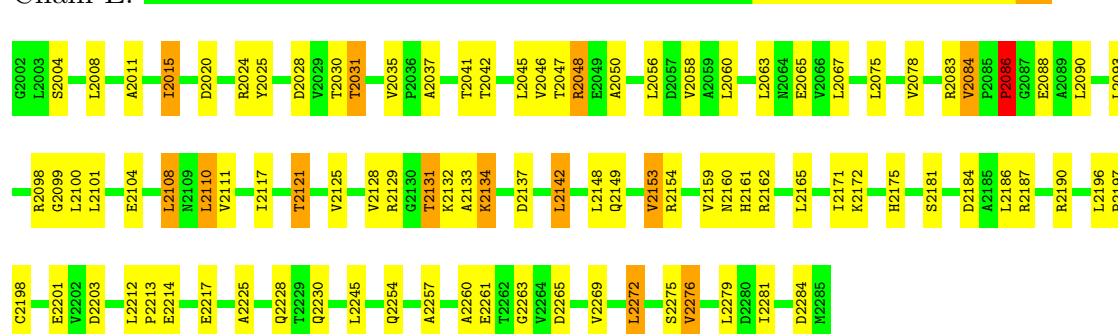
• Molecule 1: QUINOLINATE PHOSPHORIBOSYLTRANSFERASE

Chain D:



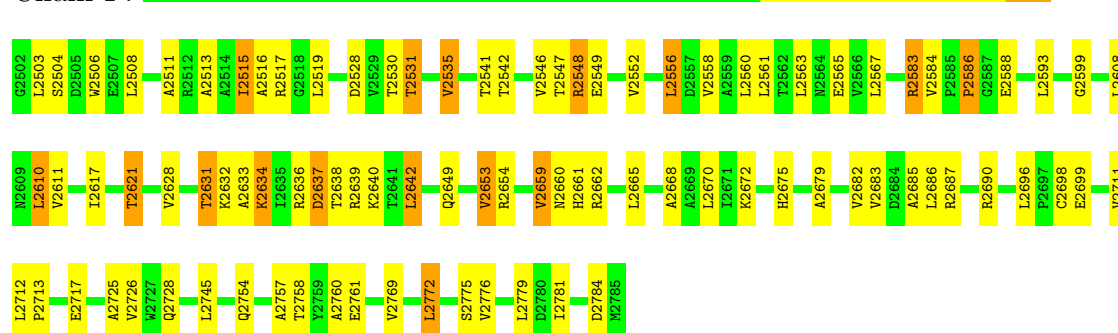
• Molecule 1: QUINOLINATE PHOSPHORIBOSYLTRANSFERASE

Chain E:



• Molecule 1: QUINOLINATE PHOSPHORIBOSYLTRANSFERASE

Chain F:



4 Data and refinement statistics

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	100.34Å 100.34Å 145.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.45	Depositor
% Data completeness (in resolution range)	97.8 (8.00-2.45)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.178 , 0.253	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12938	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: NTM, 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	0.67	0/2120	0.86	1/2891 (0.0%)
1	B	0.66	0/2120	0.86	1/2891 (0.0%)
1	C	0.68	0/2120	0.88	1/2891 (0.0%)
1	D	0.66	0/2120	0.86	1/2891 (0.0%)
1	E	0.67	0/2120	0.86	1/2891 (0.0%)
1	F	0.66	0/2120	0.86	0/2891
All	All	0.67	0/12720	0.86	5/17346 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1154	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	A	42	THR	N-CA-C	-5.80	95.33	111.00
1	B	542	THR	N-CA-C	-5.53	96.06	111.00
1	D	1542	THR	N-CA-C	-5.40	96.43	111.00
1	E	2045	LEU	CA-CB-CG	5.30	127.48	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2095	0	2135	67	0
1	B	2095	0	2135	61	0
1	C	2095	0	2135	76	0
1	D	2095	0	2135	64	0
1	E	2095	0	2135	65	0
1	F	2095	0	2135	67	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	12	0	3	0	0
3	B	12	0	3	1	0
3	C	12	0	3	0	0
3	D	12	0	3	0	0
3	E	12	0	3	1	0
3	F	12	0	3	2	0
4	A	36	0	0	1	0
4	B	47	0	0	2	0
4	C	60	0	0	8	0
4	D	43	0	0	1	0
4	E	47	0	0	3	0
4	F	33	0	0	0	0
All	All	12938	0	12828	366	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (366) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:67:LEU:HD21	1:A:99:GLY:HA3	1.36	1.02
1:C:1175:HIS:HE1	1:D:1531:THR:HG22	1.23	1.02
1:E:2031:THR:HG22	1:F:2675:HIS:HE1	1.30	0.95
1:E:2175:HIS:HE1	1:F:2531:THR:HG22	1.30	0.94
1:C:1175:HIS:CE1	1:D:1531:THR:HG22	2.06	0.91
1:A:131:THR:HG21	1:A:260:ALA:HB1	1.54	0.90
1:C:1031:THR:HG22	1:D:1675:HIS:HE1	1.32	0.90
1:D:1631:THR:HG21	1:D:1760:ALA:HB1	1.51	0.90
1:B:567:LEU:HD21	1:B:599:GLY:HA3	1.53	0.89
1:D:1515:ILE:HD11	1:D:1565:GLU:HG2	1.53	0.89
1:E:2131:THR:HG21	1:E:2260:ALA:HB1	1.55	0.88
1:E:2067:LEU:HD21	1:E:2099:GLY:HA3	1.55	0.88

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:175:HIS:HE1	1:B:531:THR:HG22	1.39	0.87
1:C:1031:THR:HG22	1:D:1675:HIS:CE1	2.14	0.82
1:E:2031:THR:HG22	1:F:2675:HIS:CE1	2.14	0.81
1:E:2175:HIS:CE1	1:F:2531:THR:HG22	2.14	0.81
1:B:631:THR:HG21	1:B:760:ALA:HB1	1.61	0.80
1:D:1567:LEU:HD21	1:D:1599:GLY:HA3	1.64	0.80
1:F:2515:ILE:HD11	1:F:2565:GLU:HG2	1.64	0.79
1:B:725:ALA:H	1:B:728:GLN:HE21	1.32	0.78
1:D:1672:LYS:H	1:D:1675:HIS:HD2	1.30	0.78
1:C:1046:VAL:HG22	1:C:1048:ARG:HH21	1.48	0.77
1:A:225:ALA:H	1:A:228:GLN:HE21	1.32	0.77
1:C:1225:ALA:H	1:C:1228:GLN:HE21	1.30	0.77
1:A:84:VAL:HG22	1:A:88:GLU:HG2	1.66	0.77
1:A:172:LYS:H	1:A:175:HIS:HD2	1.31	0.76
1:C:1172:LYS:H	1:C:1175:HIS:HD2	1.33	0.76
1:C:1015:ILE:HD11	1:C:1065:GLU:HG2	1.67	0.76
1:B:632:LYS:O	1:B:634:LYS:HE2	1.87	0.74
1:C:1276:VAL:O	1:D:1775:SER:HA	1.88	0.73
1:E:2121:THR:HG21	1:E:2153:VAL:HA	1.70	0.73
1:C:1225:ALA:H	1:C:1228:GLN:NE2	1.87	0.73
1:A:175:HIS:CE1	1:B:531:THR:HG22	2.23	0.73
1:F:2725:ALA:H	1:F:2728:GLN:HE21	1.38	0.72
1:E:2132:LYS:O	1:E:2134:LYS:HE2	1.90	0.71
1:D:1632:LYS:O	1:D:1634:LYS:HE2	1.91	0.71
1:E:2172:LYS:H	1:E:2175:HIS:HD2	1.38	0.71
1:D:1515:ILE:HD11	1:D:1565:GLU:CG	2.22	0.70
1:C:1048:ARG:HD3	4:C:3220:HOH:O	1.92	0.69
1:B:672:LYS:H	1:B:675:HIS:HD2	1.39	0.68
1:D:1503:LEU:HB2	1:D:1508:LEU:HD13	1.74	0.68
1:E:2225:ALA:H	1:E:2228:GLN:HE21	1.39	0.68
1:C:1132:LYS:O	1:C:1134:LYS:HE2	1.93	0.68
1:A:67:LEU:CD2	1:A:99:GLY:HA3	2.20	0.68
1:F:2621:THR:HG21	1:F:2653:VAL:HA	1.75	0.68
1:C:1201:GLU:HG3	1:C:1220:LEU:HD22	1.76	0.67
1:F:2631:THR:HG23	1:F:2633:ALA:H	1.59	0.67
1:D:1621:THR:HG21	1:D:1653:VAL:HA	1.77	0.67
1:D:1654:ARG:HE	1:D:1660:ASN:ND2	1.92	0.67
1:F:2661:HIS:HD2	1:F:2662:ARG:H	1.42	0.67
1:A:31:THR:HG22	1:B:675:HIS:HE1	1.61	0.66
1:A:15:ILE:HD11	1:A:65:GLU:HG2	1.77	0.66
1:F:2584:VAL:HG22	1:F:2588:GLU:HG2	1.77	0.66
1:A:131:THR:HG23	1:A:133:ALA:H	1.59	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:725:ALA:H	1:B:728:GLN:NE2	1.93	0.66
1:F:2661:HIS:CD2	1:F:2662:ARG:H	2.13	0.66
1:C:1076:ASP:HB3	4:C:3250:HOH:O	1.95	0.66
1:C:1275:SER:HA	1:D:1776:VAL:O	1.95	0.66
1:E:2275:SER:HA	1:F:2776:VAL:O	1.96	0.66
1:E:2131:THR:HG23	1:E:2133:ALA:H	1.61	0.65
1:C:1067:LEU:HD21	1:C:1099:GLY:HA3	1.77	0.65
1:F:2672:LYS:H	1:F:2675:HIS:HD2	1.43	0.65
1:D:1725:ALA:H	1:D:1728:GLN:HE21	1.42	0.65
1:D:1639:ARG:NH2	4:D:3005:HOH:O	2.30	0.65
1:C:1011:ALA:O	1:C:1015:ILE:HG23	1.97	0.65
1:D:1550:ALA:HB2	1:D:1586:PRO:HD3	1.79	0.64
1:E:2134:LYS:HE3	1:E:2265:ASP:O	1.98	0.64
1:F:2637:ASP:OD2	1:F:2653:VAL:HG21	1.97	0.64
1:B:515:ILE:HD11	1:B:565:GLU:HG2	1.79	0.64
1:D:1584:VAL:HG22	1:D:1588:GLU:HG2	1.80	0.64
1:D:1634:LYS:HE3	1:D:1765:ASP:O	1.97	0.64
1:D:1632:LYS:HE2	1:D:1763:GLY:O	1.97	0.64
1:C:1154:ARG:HE	1:C:1160:ASN:ND2	1.96	0.64
1:E:2046:VAL:HG22	1:E:2048:ARG:HH21	1.63	0.64
1:F:2567:LEU:HD21	1:F:2599:GLY:HA3	1.80	0.63
1:A:117:ILE:O	1:A:121:THR:HG23	1.98	0.63
1:E:2225:ALA:H	1:E:2228:GLN:NE2	1.96	0.63
1:A:121:THR:HG21	1:A:153:VAL:HA	1.79	0.62
1:A:275:SER:HA	1:B:776:VAL:O	1.98	0.62
1:A:225:ALA:H	1:A:228:GLN:NE2	1.96	0.62
1:E:2028:ASP:CG	1:E:2031:THR:HG23	2.20	0.62
1:F:2632:LYS:O	1:F:2634:LYS:HE2	2.00	0.62
1:E:2276:VAL:O	1:F:2775:SER:HA	2.00	0.62
1:C:1131:THR:HG21	1:C:1260:ALA:HB1	1.81	0.62
1:A:198:CYS:O	1:A:217:GLU:HB2	2.00	0.62
1:D:1654:ARG:HE	1:D:1660:ASN:HD21	1.48	0.62
1:C:1196:LEU:CD2	1:D:1529:VAL:HG11	2.30	0.62
1:A:276:VAL:O	1:B:775:SER:HA	2.00	0.61
1:F:2547:THR:HG22	1:F:2781:ILE:HG12	1.81	0.61
1:E:2047:THR:HG22	1:E:2281:ILE:HG12	1.83	0.61
1:F:2528:ASP:CG	1:F:2531:THR:HG23	2.20	0.61
1:C:1024:ARG:HD3	4:C:3229:HOH:O	2.01	0.61
1:A:212:LEU:N	1:A:213:PRO:HD2	2.15	0.61
1:C:1234:GLN:NE2	4:C:3168:HOH:O	2.33	0.61
1:D:1725:ALA:H	1:D:1728:GLN:NE2	1.99	0.60
1:A:31:THR:HG22	1:B:675:HIS:CE1	2.36	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:631:THR:CG2	1:B:633:ALA:H	2.15	0.60
1:F:2631:THR:HG21	1:F:2760:ALA:HB1	1.83	0.60
1:D:1546:VAL:HG22	1:D:1548:ARG:HH21	1.66	0.60
1:A:131:THR:CG2	1:A:133:ALA:H	2.14	0.60
1:C:1117:ILE:O	1:C:1121:THR:HG23	2.02	0.60
1:B:504:SER:H	1:B:507:GLU:HB2	1.66	0.59
1:C:1131:THR:HG23	1:C:1133:ALA:H	1.67	0.59
1:B:584:VAL:HG22	1:B:588:GLU:HG2	1.84	0.59
1:E:2015:ILE:HD11	1:E:2065:GLU:HG2	1.85	0.59
1:F:2712:LEU:N	1:F:2713:PRO:HD2	2.18	0.59
1:E:2142:LEU:H	1:E:2149:GLN:HE22	1.51	0.58
1:E:2058:VAL:HG11	1:E:2110:LEU:HG	1.84	0.58
1:A:28:ASP:CG	1:A:31:THR:HG23	2.22	0.58
1:C:1028:ASP:CG	1:C:1031:THR:HG23	2.24	0.58
1:B:621:THR:HG21	1:B:653:VAL:HA	1.85	0.58
1:A:229:THR:O	1:A:233:VAL:HG23	2.03	0.58
1:B:631:THR:HG23	1:B:633:ALA:H	1.68	0.58
1:E:2084:VAL:HG22	1:E:2088:GLU:HG2	1.85	0.58
1:C:1198:CYS:O	1:C:1217:GLU:HB2	2.04	0.58
1:C:1047:THR:O	1:C:1086:PRO:O	2.21	0.57
1:C:1161:HIS:CD2	1:C:1162:ARG:H	2.23	0.57
1:D:1662:ARG:HB2	1:D:1667:ASP:HB3	1.87	0.57
1:C:1190:ARG:NH1	4:C:3025:HOH:O	2.37	0.57
1:D:1504:SER:O	1:D:1508:LEU:HB2	2.05	0.56
1:A:196:LEU:CD2	1:B:529:VAL:HG11	2.36	0.56
1:F:2558:VAL:HG11	1:F:2610:LEU:HG	1.85	0.56
1:A:50:ALA:HB2	1:A:86:PRO:HD3	1.87	0.56
1:E:2129:ARG:HD2	4:E:3130:HOH:O	2.05	0.56
1:D:1528:ASP:CG	1:D:1531:THR:HG23	2.25	0.56
1:B:528:ASP:CG	1:B:531:THR:HG23	2.25	0.56
1:D:1712:LEU:N	1:D:1713:PRO:HD2	2.20	0.56
1:D:1515:ILE:HD11	1:D:1565:GLU:CB	2.36	0.56
1:A:4:SER:O	1:A:8:LEU:HB2	2.06	0.56
1:B:661:HIS:CE1	3:B:2902:NTM:H4	2.41	0.56
1:A:154:ARG:HE	1:A:160:ASN:ND2	2.04	0.56
1:B:632:LYS:HE2	1:B:763:GLY:O	2.06	0.56
1:F:2515:ILE:HD11	1:F:2565:GLU:CG	2.33	0.55
1:A:201:GLU:HG3	1:A:220:LEU:HD22	1.88	0.55
1:A:128:VAL:O	1:A:131:THR:HB	2.05	0.55
1:C:1121:THR:HG21	1:C:1153:VAL:HA	1.87	0.55
1:D:1661:HIS:CD2	1:D:1662:ARG:H	2.24	0.55
1:E:2131:THR:CG2	1:E:2133:ALA:H	2.18	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:2617:ILE:O	1:F:2621:THR:HG23	2.07	0.55
1:E:2212:LEU:N	1:E:2213:PRO:HD2	2.21	0.55
1:B:617:ILE:O	1:B:621:THR:HG23	2.06	0.55
1:B:712:LEU:N	1:B:713:PRO:HD2	2.21	0.55
1:B:567:LEU:CD2	1:B:599:GLY:HA3	2.32	0.55
1:A:117:ILE:O	1:A:121:THR:CG2	2.55	0.55
1:A:269:VAL:HB	1:A:272:LEU:HD22	1.88	0.55
1:E:2117:ILE:O	1:E:2121:THR:HG23	2.07	0.54
1:A:143:PRO:HG3	1:B:610:LEU:HD21	1.89	0.54
1:C:1181:SER:HB3	1:C:1184:ASP:OD2	2.07	0.54
1:B:547:THR:O	1:B:586:PRO:O	2.26	0.54
1:C:1172:LYS:H	1:C:1175:HIS:CD2	2.21	0.54
1:B:661:HIS:CD2	1:B:662:ARG:H	2.25	0.54
1:F:2515:ILE:HG13	1:F:2516:ALA:N	2.23	0.54
1:C:1121:THR:O	1:C:1125:VAL:HG23	2.08	0.54
1:E:2161:HIS:CD2	1:E:2162:ARG:H	2.24	0.54
1:A:161:HIS:CD2	1:A:162:ARG:H	2.26	0.54
1:B:546:VAL:HG22	1:B:548:ARG:HH21	1.72	0.54
1:C:1037:ALA:HA	1:C:1098:ARG:HD2	1.89	0.53
1:E:2117:ILE:O	1:E:2121:THR:CG2	2.56	0.53
1:A:143:PRO:HG3	1:B:610:LEU:CD2	2.38	0.53
1:B:628:VAL:O	1:B:631:THR:HB	2.08	0.53
1:C:1024:ARG:NH2	1:D:1506:TRP:CH2	2.76	0.53
1:E:2037:ALA:HA	1:E:2098:ARG:HD2	1.90	0.53
1:B:634:LYS:HE3	1:B:765:ASP:O	2.09	0.53
1:D:1642:LEU:H	1:D:1649:GLN:HE22	1.55	0.53
1:D:1661:HIS:HD2	1:D:1662:ARG:H	1.57	0.53
1:A:143:PRO:HD3	4:A:3260:HOH:O	2.08	0.53
1:C:1239:ARG:NH1	4:C:3123:HOH:O	2.42	0.53
1:E:2011:ALA:O	1:E:2015:ILE:HG23	2.10	0.52
1:F:2725:ALA:H	1:F:2728:GLN:NE2	2.05	0.52
1:A:132:LYS:O	1:A:134:LYS:HE2	2.10	0.52
1:F:2654:ARG:HE	1:F:2660:ASN:HD21	1.56	0.52
1:A:46:VAL:HG22	1:A:48:ARG:HH21	1.75	0.52
1:D:1617:ILE:O	1:D:1621:THR:HG23	2.10	0.52
1:A:186:LEU:O	1:A:190:ARG:HG2	2.09	0.52
1:B:547:THR:HG22	1:B:781:ILE:HG12	1.90	0.52
1:E:2028:ASP:OD2	1:E:2031:THR:HG23	2.10	0.52
1:A:42:THR:HA	1:A:93:LEU:O	2.09	0.52
1:F:2504:SER:O	1:F:2508:LEU:HB2	2.10	0.51
1:F:2698:CYS:O	1:F:2717:GLU:HB2	2.10	0.51
1:E:2104:GLU:HG2	1:E:2108:LEU:HD22	1.93	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:1628:VAL:O	1:D:1631:THR:HB	2.09	0.51
1:F:2511:ALA:O	1:F:2515:ILE:HG23	2.08	0.51
1:C:1186:LEU:O	1:C:1190:ARG:HG2	2.10	0.51
1:B:698:CYS:O	1:B:717:GLU:HB2	2.11	0.51
1:C:1154:ARG:HE	1:C:1160:ASN:HD21	1.59	0.51
1:A:154:ARG:HE	1:A:160:ASN:HD21	1.57	0.51
1:B:757:ALA:O	1:B:761:GLU:HG3	2.11	0.51
1:C:1212:LEU:N	1:C:1213:PRO:HD2	2.26	0.51
1:E:2128:VAL:O	1:E:2131:THR:HB	2.11	0.51
1:D:1686:LEU:O	1:D:1690:ARG:HG2	2.10	0.51
1:A:257:ALA:O	1:A:261:GLU:HG3	2.11	0.51
1:D:1528:ASP:OD2	1:D:1531:THR:HG23	2.11	0.50
1:A:226:VAL:HG11	1:A:258:THR:HG22	1.92	0.50
1:F:2654:ARG:HE	1:F:2660:ASN:ND2	2.09	0.50
1:B:661:HIS:HD2	1:B:662:ARG:H	1.60	0.50
1:E:2181:SER:HB3	1:E:2184:ASP:OD2	2.11	0.50
1:B:672:LYS:H	1:B:675:HIS:CD2	2.26	0.50
1:E:2047:THR:HG23	1:E:2090:LEU:HD11	1.93	0.50
1:E:2050:ALA:HB2	1:E:2086:PRO:HD3	1.92	0.50
1:D:1631:THR:HG23	1:D:1633:ALA:H	1.75	0.50
1:C:1128:VAL:O	1:C:1131:THR:HB	2.11	0.50
1:D:1542:THR:HA	1:D:1593:LEU:O	2.12	0.50
1:B:524:ARG:HD2	1:B:525:TYR:CZ	2.48	0.49
1:C:1029:VAL:HG11	1:D:1696:LEU:CD2	2.42	0.49
1:B:662:ARG:HB2	1:B:667:ASP:HB3	1.93	0.49
1:B:642:LEU:H	1:B:649:GLN:HE22	1.60	0.49
1:C:1131:THR:CG2	1:C:1133:ALA:H	2.25	0.49
1:C:1035:VAL:HG22	1:C:1098:ARG:HG3	1.94	0.49
1:A:134:LYS:HE3	1:A:265:ASP:O	2.13	0.49
1:C:1047:THR:HG22	1:C:1281:ILE:HG12	1.94	0.49
1:C:1226:VAL:HG11	1:C:1258:THR:HG22	1.95	0.49
1:D:1769:VAL:HB	1:D:1772:LEU:HD22	1.94	0.49
1:C:1084:VAL:HG22	1:C:1088:GLU:HG2	1.95	0.49
1:E:2161:HIS:CE1	3:E:2905:NTM:H4	2.48	0.49
1:F:2642:LEU:H	1:F:2649:GLN:HE22	1.61	0.48
1:D:1631:THR:CG2	1:D:1633:ALA:H	2.26	0.48
1:F:2503:LEU:HB2	1:F:2508:LEU:HD13	1.95	0.48
1:F:2515:ILE:HD11	1:F:2565:GLU:CB	2.43	0.48
1:E:2161:HIS:HD2	1:E:2162:ARG:H	1.61	0.48
1:D:1672:LYS:H	1:D:1675:HIS:CD2	2.20	0.48
1:A:35:VAL:HG22	1:A:98:ARG:HG3	1.95	0.48
1:C:1161:HIS:HD2	1:C:1162:ARG:H	1.60	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:47:THR:O	1:A:86:PRO:O	2.32	0.48
1:B:550:ALA:HB2	1:B:586:PRO:HD3	1.96	0.48
1:E:2121:THR:O	1:E:2125:VAL:HG23	2.13	0.48
1:C:1136:ARG:HG2	1:C:1159:VAL:HG22	1.96	0.48
1:F:2617:ILE:O	1:F:2621:THR:CG2	2.62	0.47
1:C:1187:ARG:HH22	1:C:1190:ARG:NH2	2.12	0.47
1:B:617:ILE:O	1:B:621:THR:CG2	2.62	0.47
1:E:2257:ALA:O	1:E:2261:GLU:HG3	2.13	0.47
1:F:2513:ALA:O	1:F:2517:ARG:HG3	2.14	0.47
1:E:2269:VAL:HB	1:E:2272:LEU:HD22	1.96	0.47
1:A:87:GLY:HA3	1:E:2230:GLN:HB3	1.96	0.46
1:F:2672:LYS:H	1:F:2675:HIS:CD2	2.30	0.46
1:D:1548:ARG:NH2	1:D:1784:ASP:OD2	2.47	0.46
1:E:2154:ARG:HE	1:E:2160:ASN:ND2	2.14	0.46
1:B:701:GLU:HG3	1:B:720:LEU:HD22	1.96	0.46
1:C:1060:LEU:HD21	1:C:1091:MET:HE2	1.96	0.46
1:A:136:ARG:HG2	1:A:159:VAL:HG22	1.97	0.46
1:F:2552:VAL:HG22	1:F:2583:ARG:HG2	1.97	0.46
1:C:1015:ILE:HD11	1:C:1065:GLU:CG	2.42	0.46
1:C:1058:VAL:HG11	1:C:1110:LEU:HG	1.96	0.46
1:A:41:THR:O	1:A:94:GLU:HA	2.15	0.46
1:F:2546:VAL:HG22	1:F:2548:ARG:HH21	1.80	0.46
1:F:2508:LEU:HD12	1:F:2561:LEU:HD11	1.97	0.46
1:E:2004:SER:O	1:E:2008:LEU:HB2	2.16	0.45
1:B:513:ALA:O	1:B:517:ARG:HG3	2.16	0.45
1:E:2067:LEU:CD2	1:E:2099:GLY:HA3	2.38	0.45
1:C:1031:THR:CG2	1:D:1675:HIS:HE1	2.18	0.45
1:D:1617:ILE:O	1:D:1621:THR:CG2	2.65	0.45
1:F:2668:ALA:HA	1:F:2696:LEU:HG	1.98	0.45
1:F:2686:LEU:O	1:F:2690:ARG:HG2	2.16	0.45
1:F:2548:ARG:NH2	1:F:2784:ASP:OD2	2.50	0.45
1:C:1008:LEU:HA	1:C:1008:LEU:HD12	1.87	0.45
1:C:1148:LEU:O	1:C:1151:TYR:HB3	2.17	0.45
1:F:2670:LEU:HG	1:F:2699:GLU:HB2	1.98	0.45
1:C:1028:ASP:OD2	1:C:1031:THR:HG23	2.17	0.45
1:D:1515:ILE:CD1	1:D:1565:GLU:HG2	2.36	0.45
1:F:2639:ARG:HG3	3:F:2906:NTM:O4	2.17	0.45
1:B:654:ARG:HE	1:B:660:ASN:ND2	2.15	0.45
1:E:2020:ASP:OD2	1:E:2024:ARG:NH2	2.50	0.44
1:E:2025:TYR:N	1:E:2025:TYR:CD1	2.85	0.44
1:B:548:ARG:NH2	1:B:784:ASP:OD2	2.51	0.44
1:B:686:LEU:O	1:B:690:ARG:HG2	2.17	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:542:THR:HA	1:B:593:LEU:O	2.17	0.44
1:C:1154:ARG:HH21	1:C:1160:ASN:HD21	1.64	0.44
1:F:2542:THR:HA	1:F:2593:LEU:O	2.18	0.44
1:A:172:LYS:H	1:A:175:HIS:CD2	2.22	0.44
1:E:2024:ARG:NH2	1:F:2506:TRP:CH2	2.85	0.44
1:E:2148:LEU:HA	1:E:2148:LEU:HD23	1.83	0.44
1:F:2679:ALA:HB3	1:F:2685:ALA:HB2	2.00	0.44
1:C:1148:LEU:HD23	1:C:1148:LEU:HA	1.82	0.44
1:D:1683:VAL:O	1:D:1687:ARG:HG2	2.18	0.44
1:E:2203:ASP:HB2	4:E:3246:HOH:O	2.17	0.44
1:D:1520:ASP:OD2	1:D:1524:ARG:NH2	2.51	0.43
1:D:1535:VAL:HG22	1:D:1598:ARG:HG3	1.99	0.43
1:E:2196:LEU:HA	1:E:2197:PRO:HD3	1.91	0.43
1:B:504:SER:N	1:B:507:GLU:OE1	2.51	0.43
1:C:1225:ALA:N	1:C:1228:GLN:HE21	2.06	0.43
1:E:2132:LYS:HE2	1:E:2263:GLY:O	2.19	0.43
1:F:2610:LEU:HA	1:F:2610:LEU:HD13	1.83	0.43
1:A:28:ASP:OD2	1:A:31:THR:CG2	2.67	0.43
1:B:511:ALA:O	1:B:515:ILE:HG23	2.19	0.43
1:A:132:LYS:HE2	1:A:263:GLY:O	2.18	0.43
1:A:63:LEU:HB3	1:A:72:TYR:CE2	2.54	0.43
1:A:11:ALA:O	1:A:15:ILE:HG23	2.18	0.43
1:F:2779:LEU:HD12	1:F:2779:LEU:HA	1.78	0.43
1:B:541:THR:O	1:B:594:GLU:HA	2.18	0.43
1:E:2048:ARG:NH2	1:E:2284:ASP:OD2	2.52	0.43
1:E:2025:TYR:HB2	4:E:3179:HOH:O	2.18	0.43
1:F:2682:VAL:CG1	1:F:2711:VAL:HG11	2.48	0.43
1:D:1701:GLU:HG3	1:D:1720:LEU:HD22	2.00	0.43
1:A:187:ARG:HH22	1:A:190:ARG:NE	2.17	0.43
1:D:1547:THR:HG22	1:D:1781:ILE:HG12	2.00	0.43
1:E:2042:THR:HA	1:E:2093:LEU:O	2.19	0.43
1:B:535:VAL:HG22	1:B:598:ARG:HG3	2.01	0.43
1:C:1178:ALA:HB2	4:C:3249:HOH:O	2.19	0.43
1:F:2683:VAL:O	1:F:2687:ARG:HG2	2.19	0.42
1:C:1196:LEU:HD21	1:D:1529:VAL:HG11	1.99	0.42
1:C:1117:ILE:O	1:C:1121:THR:CG2	2.66	0.42
1:A:187:ARG:NH2	1:A:190:ARG:NE	2.67	0.42
1:E:2279:LEU:HA	1:E:2279:LEU:HD12	1.87	0.42
1:A:29:VAL:HG11	1:B:696:LEU:CD2	2.48	0.42
1:E:2198:CYS:O	1:E:2217:GLU:HB2	2.19	0.42
1:E:2137:ASP:OD2	1:E:2153:VAL:HG21	2.18	0.42
1:B:779:LEU:HA	1:B:779:LEU:HD12	1.75	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:142:LEU:H	1:A:149:GLN:HE22	1.65	0.42
1:D:1642:LEU:H	1:D:1649:GLN:NE2	2.17	0.42
1:E:2028:ASP:OD2	1:E:2031:THR:CG2	2.67	0.42
1:C:1187:ARG:HH22	1:C:1190:ARG:CZ	2.33	0.42
1:E:2186:LEU:O	1:E:2190:ARG:HG2	2.19	0.42
1:F:2636:ARG:HG2	1:F:2659:VAL:HG22	2.01	0.42
1:D:1515:ILE:HG13	1:D:1516:ALA:N	2.33	0.42
1:A:56:LEU:O	1:A:59:ALA:HB3	2.20	0.42
1:D:1702:VAL:HA	1:D:1707:GLN:OE1	2.19	0.42
1:E:2100:LEU:HA	1:E:2100:LEU:HD23	1.89	0.42
1:F:2726:VAL:HG11	1:F:2758:THR:HG22	2.02	0.42
1:E:2142:LEU:H	1:E:2149:GLN:NE2	2.16	0.42
1:A:37:ALA:HA	1:A:98:ARG:HD2	2.01	0.42
1:A:58:VAL:HG11	1:A:110:LEU:HG	2.02	0.42
1:F:2757:ALA:O	1:F:2761:GLU:HG3	2.19	0.42
1:D:1698:CYS:O	1:D:1717:GLU:HB2	2.20	0.42
1:F:2531:THR:O	1:F:2535:VAL:HG13	2.19	0.41
1:B:525:TYR:HE1	4:B:3066:HOH:O	2.02	0.41
1:C:1196:LEU:HA	1:C:1197:PRO:HD3	1.94	0.41
1:F:2631:THR:CG2	1:F:2633:ALA:H	2.31	0.41
1:B:515:ILE:HD11	1:B:565:GLU:CG	2.48	0.41
1:C:1162:ARG:HB2	1:C:1167:ASP:HB3	2.02	0.41
1:F:2687:ARG:HH22	1:F:2690:ARG:CZ	2.34	0.41
1:E:2190:ARG:NH2	1:E:2214:GLU:O	2.53	0.41
1:D:1528:ASP:OD2	1:D:1531:THR:CG2	2.68	0.41
1:A:190:ARG:NH2	1:A:214:GLU:O	2.53	0.41
1:A:181:SER:HB3	1:A:184:ASP:OD2	2.21	0.41
1:C:1056:LEU:HA	1:C:1056:LEU:HD12	1.90	0.41
1:F:2515:ILE:HD12	1:F:2519:LEU:HD12	2.03	0.41
1:B:687:ARG:HH22	1:B:690:ARG:NH2	2.19	0.41
1:C:1134:LYS:HG2	4:C:3037:HOH:O	2.21	0.41
1:F:2628:VAL:O	1:F:2631:THR:HB	2.20	0.41
1:D:1637:ASP:OD2	1:D:1653:VAL:HG21	2.21	0.41
1:A:277:ARG:HA	1:B:775:SER:HA	2.03	0.41
1:D:1524:ARG:HD2	1:D:1525:TYR:CZ	2.55	0.41
1:F:2769:VAL:HB	1:F:2772:LEU:HD22	2.03	0.41
1:C:1271:ALA:HA	1:C:1274:HIS:CE1	2.56	0.41
1:B:722:ASP:O	1:B:723:ASN:HB2	2.21	0.41
1:A:230:GLN:HB3	1:C:1087:GLY:HA3	2.02	0.41
1:F:2556:LEU:HD12	1:F:2556:LEU:HA	1.96	0.41
1:A:136:ARG:HA	1:A:159:VAL:O	2.21	0.41
1:E:2187:ARG:NH2	1:E:2190:ARG:NE	2.68	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:1646:ARG:O	1:D:1650:LYS:HB2	2.21	0.41
1:F:2547:THR:HB	1:F:2549:GLU:O	2.21	0.40
1:A:25:TYR:HE2	4:B:3158:HOH:O	2.03	0.40
1:A:196:LEU:HD21	1:B:529:VAL:HG11	2.03	0.40
1:C:1100:LEU:HD23	1:C:1100:LEU:HA	1.93	0.40
1:C:1019:LEU:HD23	1:C:1019:LEU:HA	1.90	0.40
1:F:2649:GLN:O	1:F:2653:VAL:HG13	2.21	0.40
1:C:1136:ARG:HA	1:C:1159:VAL:O	2.21	0.40
1:A:29:VAL:HG11	1:B:696:LEU:HD23	2.02	0.40
1:C:1143:PRO:HG3	1:D:1610:LEU:HD21	2.02	0.40
1:D:1757:ALA:O	1:D:1761:GLU:HG3	2.20	0.40
1:C:1134:LYS:HE3	1:C:1265:ASP:O	2.21	0.40
1:C:1279:LEU:HA	1:C:1279:LEU:HD12	1.91	0.40
1:F:2638:THR:OG1	1:F:2640:LYS:HG3	2.22	0.40
1:E:2171:ILE:O	1:E:2201:GLU:HB3	2.22	0.40
1:F:2528:ASP:OD2	1:F:2531:THR:CG2	2.70	0.40
1:F:2661:HIS:CE1	3:F:2906:NTM:H5	2.57	0.40
1:C:1142:LEU:H	1:C:1149:GLN:HE22	1.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	282/284 (99%)	276 (98%)	5 (2%)	1 (0%)	43	64
1	B	282/284 (99%)	275 (98%)	6 (2%)	1 (0%)	43	64
1	C	282/284 (99%)	276 (98%)	5 (2%)	1 (0%)	43	64
1	D	282/284 (99%)	274 (97%)	7 (2%)	1 (0%)	43	64
1	E	282/284 (99%)	274 (97%)	7 (2%)	1 (0%)	43	64
1	F	282/284 (99%)	276 (98%)	5 (2%)	1 (0%)	43	64
All	All	1692/1704 (99%)	1651 (98%)	35 (2%)	6 (0%)	43	64

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	2586	PRO
1	B	586	PRO
1	D	1586	PRO
1	E	2086	PRO
1	A	86	PRO
1	C	1086	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	216/216 (100%)	188 (87%)	28 (13%)	6	10
1	B	216/216 (100%)	191 (88%)	25 (12%)	8	13
1	C	216/216 (100%)	188 (87%)	28 (13%)	6	10
1	D	216/216 (100%)	188 (87%)	28 (13%)	6	10
1	E	216/216 (100%)	187 (87%)	29 (13%)	6	9
1	F	216/216 (100%)	191 (88%)	25 (12%)	8	13
All	All	1296/1296 (100%)	1133 (87%)	163 (13%)	7	10

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ILE
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	78	VAL
1	A	83	ARG
1	A	84	VAL

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Mol	Chain	Res	Type
1	A	86	PRO
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	153	VAL
1	A	159	VAL
1	A	165	LEU
1	A	245	LEU
1	A	254	GLN
1	A	272	LEU
1	B	515	ILE
1	B	530	THR
1	B	531	THR
1	B	535	VAL
1	B	541	THR
1	B	548	ARG
1	B	556	LEU
1	B	560	LEU
1	B	563	LEU
1	B	578	VAL
1	B	583	ARG
1	B	586	PRO
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	659	VAL
1	B	665	LEU
1	B	745	LEU
1	B	772	LEU
1	C	1015	ILE
1	C	1030	THR

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Mol	Chain	Res	Type
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	1083	ARG
1	C	1086	PRO
1	C	1101	LEU
1	C	1108	LEU
1	C	1110	LEU
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	1159	VAL
1	C	1165	LEU
1	C	1218	LEU
1	C	1245	LEU
1	C	1254	GLN
1	C	1272	LEU
1	C	1276	VAL
1	D	1515	ILE
1	D	1530	THR
1	D	1531	THR
1	D	1532	LEU
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	1583	ARG
1	D	1586	PRO
1	D	1601	LEU
1	D	1608	LEU

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Mol	Chain	Res	Type
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	1659	VAL
1	D	1665	LEU
1	D	1745	LEU
1	D	1754	GLN
1	D	1772	LEU
1	E	2015	ILE
1	E	2030	THR
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	2075	LEU
1	E	2078	VAL
1	E	2083	ARG
1	E	2084	VAL
1	E	2086	PRO
1	E	2101	LEU
1	E	2108	LEU
1	E	2110	LEU
1	E	2111	VAL
1	E	2121	THR
1	E	2131	THR
1	E	2134	LYS
1	E	2142	LEU
1	E	2153	VAL
1	E	2159	VAL
1	E	2165	LEU
1	E	2245	LEU
1	E	2254	GLN
1	E	2272	LEU
1	E	2276	VAL
1	F	2515	ILE

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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	2583	ARG
1	F	2586	PRO
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	2637	ASP
1	F	2642	LEU
1	F	2653	VAL
1	F	2659	VAL
1	F	2665	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	161	HIS
1	A	175	HIS
1	A	228	GLN
1	B	649	GLN
1	B	660	ASN
1	B	661	HIS
1	B	675	HIS
1	B	728	GLN
1	C	1149	GLN
1	C	1160	ASN
1	C	1161	HIS
1	C	1175	HIS

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Mol	Chain	Res	Type
1	C	1228	GLN
1	D	1649	GLN
1	D	1660	ASN
1	D	1661	HIS
1	D	1675	HIS
1	D	1728	GLN
1	E	2149	GLN
1	E	2160	ASN
1	E	2161	HIS
1	E	2175	HIS
1	E	2228	GLN
1	F	2649	GLN
1	F	2660	ASN
1	F	2661	HIS
1	F	2675	HIS
1	F	2728	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

12 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
3	NTM	A	2901	-	12,12,12	1.16	1 (8%)	16,16,16	1.33	1 (6%)
2	SO4	A	2985	-	4,4,4	1.78	1 (25%)	6,6,6	0.38	0
3	NTM	B	2902	-	12,12,12	0.89	1 (8%)	16,16,16	1.49	3 (18%)
2	SO4	B	2986	-	4,4,4	1.96	2 (50%)	6,6,6	0.46	0
3	NTM	C	2903	-	12,12,12	1.16	1 (8%)	16,16,16	1.59	2 (12%)
2	SO4	C	2987	-	4,4,4	2.26	3 (75%)	6,6,6	0.55	0
3	NTM	D	2904	-	12,12,12	0.99	0	16,16,16	1.36	1 (6%)
2	SO4	D	2990	-	4,4,4	2.23	2 (50%)	6,6,6	0.32	0
3	NTM	E	2905	-	12,12,12	1.32	2 (16%)	16,16,16	1.22	1 (6%)
2	SO4	E	2989	-	4,4,4	1.67	1 (25%)	6,6,6	0.41	0
3	NTM	F	2906	-	12,12,12	1.02	1 (8%)	16,16,16	1.35	2 (12%)
2	SO4	F	2988	-	4,4,4	1.41	1 (25%)	6,6,6	0.34	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
3	NTM	A	2901	-	-	0/8/8/8	0/1/1/1
2	SO4	A	2985	-	-	0/0/0/0	0/0/0/0
3	NTM	B	2902	-	-	0/8/8/8	0/1/1/1
2	SO4	B	2986	-	-	0/0/0/0	0/0/0/0
3	NTM	C	2903	-	-	0/8/8/8	0/1/1/1
2	SO4	C	2987	-	-	0/0/0/0	0/0/0/0
3	NTM	D	2904	-	-	0/8/8/8	0/1/1/1
2	SO4	D	2990	-	-	0/0/0/0	0/0/0/0
3	NTM	E	2905	-	-	0/8/8/8	0/1/1/1
2	SO4	E	2989	-	-	0/0/0/0	0/0/0/0
3	NTM	F	2906	-	-	0/8/8/8	0/1/1/1
2	SO4	F	2988	-	-	0/0/0/0	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2990	SO4	O3-S	3.36	1.58	1.47
3	C	2903	NTM	O3-C8	2.90	1.32	1.23
2	C	2987	SO4	O3-S	2.85	1.57	1.47
2	C	2987	SO4	O2-S	2.78	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2986	SO4	O3-S	2.57	1.56	1.47
3	E	2905	NTM	C2-C7	-2.56	1.47	1.51
2	A	2985	SO4	O3-S	2.42	1.55	1.47
2	D	2990	SO4	O4-S	2.40	1.55	1.47
2	B	2986	SO4	O4-S	2.27	1.55	1.47
2	E	2989	SO4	O3-S	2.27	1.55	1.47
3	F	2906	NTM	O3-C8	2.24	1.29	1.23
3	E	2905	NTM	O3-C8	2.20	1.29	1.23
2	C	2987	SO4	O4-S	2.15	1.54	1.47
3	B	2902	NTM	O3-C8	2.05	1.29	1.23
2	F	2988	SO4	O3-S	2.02	1.54	1.47
3	A	2901	NTM	C2-C7	-2.01	1.48	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2903	NTM	C6-N1-C2	3.73	123.70	116.86
3	A	2901	NTM	C6-N1-C2	3.70	123.64	116.86
3	F	2906	NTM	C6-N1-C2	3.51	123.29	116.86
3	D	2904	NTM	C6-N1-C2	3.48	123.23	116.86
3	B	2902	NTM	C6-N1-C2	3.43	123.15	116.86
3	C	2903	NTM	O2-C7-C2	3.07	122.79	114.39
3	E	2905	NTM	C6-N1-C2	3.05	122.45	116.86
3	B	2902	NTM	O2-C7-C2	2.39	120.95	114.39
3	B	2902	NTM	C4-C3-C8	-2.30	113.34	118.56
3	F	2906	NTM	O2-C7-C2	2.03	119.94	114.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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.