Full wwPDB X-ray Structure Validation Report (i)

Aug 19, 2023 – 09:22 PM EDT

PDB ID	:	2FTK
Title	:	berylloflouride Spo0F complex with Spo0B
Authors	:	Varughese, K.I.
Deposited on	:	2006-01-24
Resolution	:	3.05 Å(reported)

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

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

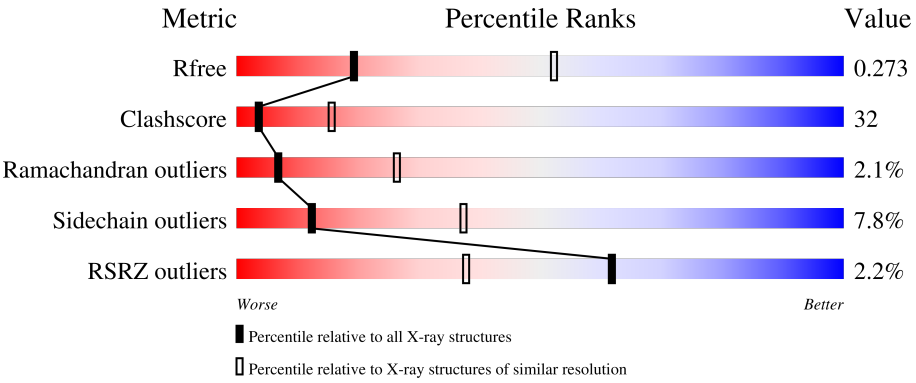
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	192	52% 39% 6%
1	B	192	48% 41% 5% 5%
1	C	192	41% 47% 5% 6%
1	D	192	48% 42% 5%
2	E	124	55% 36% 5%

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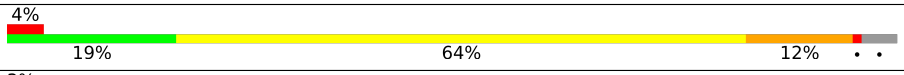
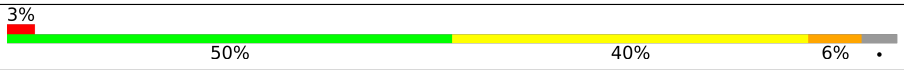
Mol	Chain	Length	Quality of chain
2	F	124	
2	G	124	
2	H	124	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9834 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 Sporulation initiation phosphotransferase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	0	0
			1497	955	251	284	7			
1	B	182	Total	C	N	O	S	6	0	0
			1505	959	253	286	7			
1	C	181	Total	C	N	O	S	0	0	0
			1497	955	251	284	7			
1	D	182	Total	C	N	O	S	6	0	0
			1505	959	253	286	7			

- Molecule 2 is a protein called Sporulation initiation phosphotransferase F.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
2	E	119	Total	Be	C	F	N	O	S	0	0	0
			954	1	609	3	156	180	5			
2	F	119	Total	Be	C	F	N	O	S	0	0	0
			954	1	609	3	156	180	5			
2	G	119	Total	Be	C	F	N	O	S	0	0	0
			954	1	609	3	156	180	5			
2	H	119	Total	Be	C	F	N	O	S	0	1	0
			964	1	615	3	159	181	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1213	SER	TYR	engineered mutation	UNP P06628
E	1254	BFD	ASP	modified residue	UNP P06628
F	1013	SER	TYR	engineered mutation	UNP P06628
F	1054	BFD	ASP	modified residue	UNP P06628
G	1613	SER	TYR	engineered mutation	UNP P06628
G	1654	BFD	ASP	modified residue	UNP P06628
H	1413	SER	TYR	engineered mutation	UNP P06628
H	1454	BFD	ASP	modified residue	UNP P06628

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

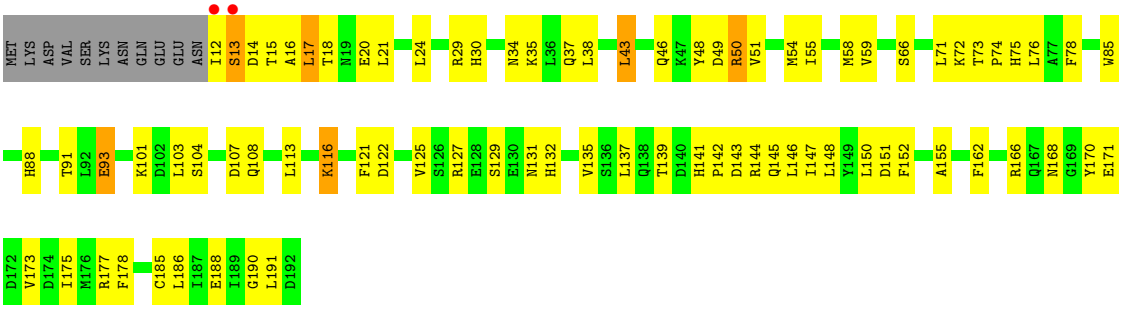
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total Mg 1 1	0	0
3	F	1	Total Mg 1 1	0	0
3	G	1	Total Mg 1 1	0	0
3	H	1	Total Mg 1 1	0	0

3 Residue-property plots (i)

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

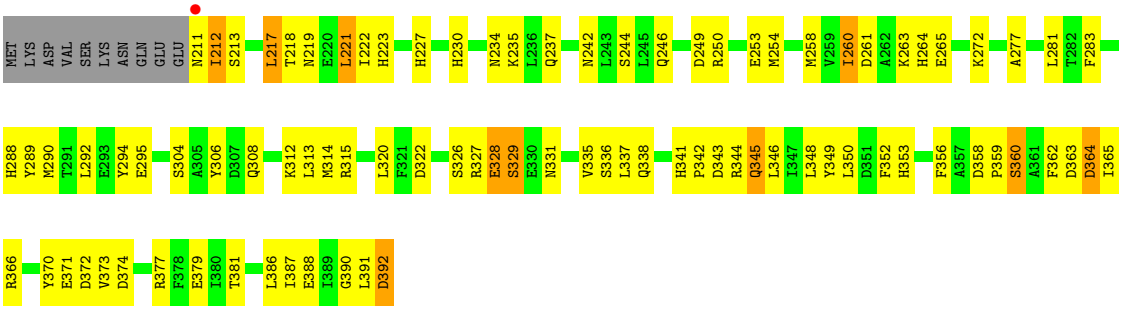
• Molecule 1: Sporulation initiation phosphotransferase B

Chain A:



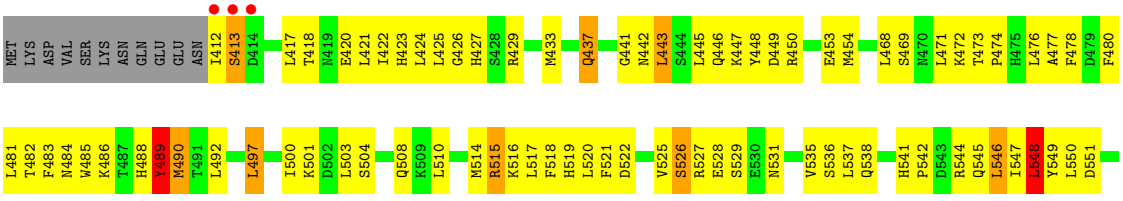
• Molecule 1: Sporulation initiation phosphotransferase B

Chain B:



• Molecule 1: Sporulation initiation phosphotransferase B

Chain C:

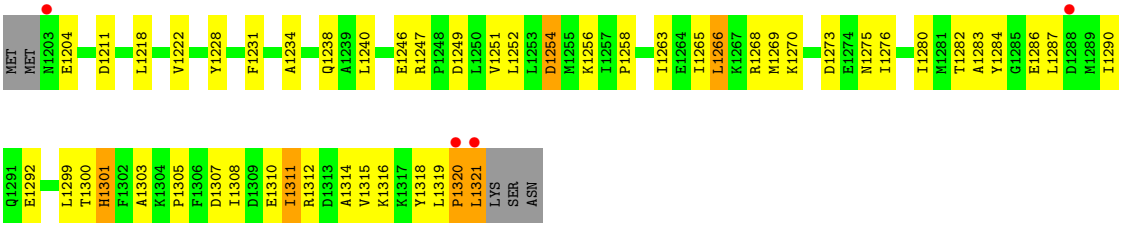


• Molecule 1: Sporulation initiation phosphotransferase B

Chain D:

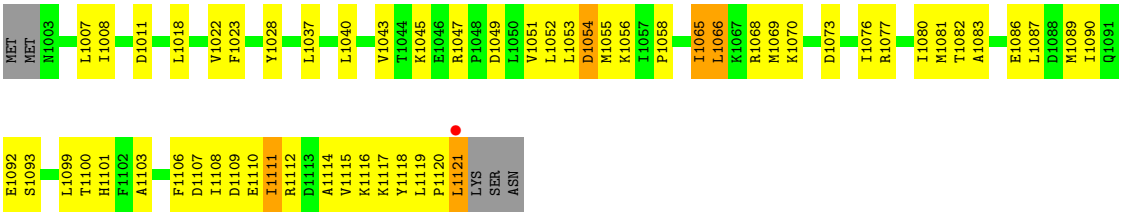
• Molecule 2: Sporulation initiation phosphotransferase F

Chain E:



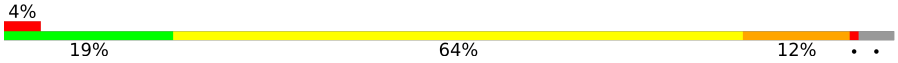
• Molecule 2: Sporulation initiation phosphotransferase F

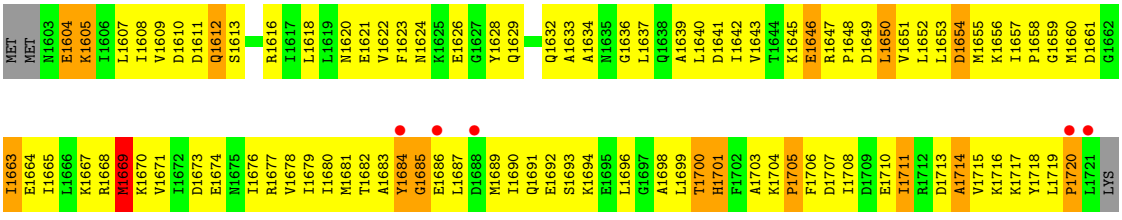
Chain F:



• Molecule 2: Sporulation initiation phosphotransferase F

Chain G:

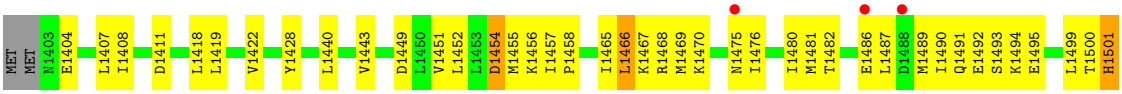




SER
ASN

• Molecule 2: Sporulation initiation phosphotransferase F

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.47Å 118.33Å 168.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.86 – 3.05 19.86 – 3.05	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.86-3.05) 98.7 (19.86-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.21 (at 3.04Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.232 , 0.282 0.222 , 0.273	Depositor DCC
R_{free} test set	1404 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	74.1	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 48.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9834	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.57	0/1530	0.67	0/2064
1	B	0.54	0/1538	0.71	0/2075
1	C	0.45	0/1530	0.66	1/2064 (0.0%)
1	D	0.44	0/1538	0.63	0/2075
2	E	0.38	0/952	0.61	0/1279
2	F	0.46	0/952	0.66	0/1279
2	G	0.32	0/952	0.61	0/1279
2	H	0.35	0/963	0.60	0/1294
All	All	0.46	0/9955	0.65	1/13409 (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	C	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	548	LEU	CA-CB-CG	5.22	127.30	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	489	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	1497	0	1457	86	0
1	B	1505	0	1463	80	0
1	C	1497	0	1457	130	0
1	D	1505	0	1463	94	0
2	E	954	0	986	43	0
2	F	954	0	986	43	0
2	G	954	0	986	136	0
2	H	964	0	992	51	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
All	All	9834	0	9790	618	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 32.

All (618) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1687:LEU:HA	2:G:1690:ILE:HD13	1.26	1.10
2:E:1251:VAL:HG11	2:E:1269:MET:HE1	1.40	1.02
1:C:565:ILE:HD12	1:C:565:ILE:H	1.25	1.01
2:G:1620:ASN:ND2	2:G:1632:GLN:HE21	1.60	0.98
1:B:381:THR:HG23	1:C:581:THR:HG23	1.48	0.94
1:A:141:HIS:HD2	1:A:144:ARG:H	1.15	0.94
1:C:437:GLN:HG2	2:G:1705:PRO:HA	1.49	0.91
2:G:1699:LEU:H	2:G:1699:LEU:HD12	1.34	0.91
2:G:1704:LYS:HA	2:G:1706:PHE:H	1.36	0.90
2:H:1451:VAL:HG11	2:H:1469:MET:HE1	1.55	0.88
1:D:678:PHE:O	1:D:682:THR:HG23	1.72	0.87
2:G:1665:ILE:HA	2:G:1668:ARG:HD3	1.58	0.85
1:C:471:LEU:HB2	1:C:473:THR:HG22	1.58	0.85
2:G:1651:VAL:HB	2:G:1678:VAL:HG22	1.59	0.84
2:G:1641:ASP:HB3	2:G:1645:LYS:HE3	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:GLY:C	1:A:191:LEU:HD12	2.00	0.82
2:G:1704:LYS:HA	2:G:1706:PHE:N	1.94	0.82
1:A:12:ILE:HG13	1:B:315:ARG:NH2	1.95	0.82
2:F:1051:VAL:HG11	2:F:1069:MET:HE1	1.60	0.82
2:H:1422:VAL:HG21	2:H:1508:ILE:HD11	1.62	0.81
1:D:773:VAL:HG12	1:D:791:LEU:HD11	1.63	0.81
1:A:24:LEU:HG	1:B:221:LEU:CD1	2.13	0.79
2:G:1714:ALA:HA	2:G:1717:LYS:HE2	1.65	0.79
1:A:71:LEU:HB2	1:A:73:THR:HG22	1.65	0.79
2:G:1613:SER:HB3	2:G:1616:ARG:HH21	1.48	0.78
1:C:545:GLN:HB2	1:C:592:ASP:HB2	1.66	0.78
1:D:709:LYS:NZ	1:D:709:LYS:HB2	1.98	0.78
1:D:649:ASP:O	1:D:653:GLU:HG3	1.84	0.77
2:G:1616:ARG:HH11	2:G:1634:ALA:HA	1.49	0.77
1:A:17:LEU:HG	1:A:21:LEU:HD11	1.65	0.77
1:C:515:ARG:HH11	1:C:515:ARG:HB2	1.49	0.76
1:C:489:TYR:CD2	1:C:490:MET:HG2	2.20	0.76
1:A:78:PHE:CD2	1:B:221:LEU:HD22	2.21	0.76
1:C:484:ASN:HD21	1:C:492:LEU:H	1.32	0.76
1:B:223:HIS:CE1	1:B:227:HIS:HE1	2.04	0.76
1:A:127:ARG:HG3	1:A:127:ARG:HH11	1.49	0.76
2:F:1022:VAL:HG21	2:F:1108:ILE:HD11	1.68	0.76
1:B:370:TYR:HD2	1:B:373:VAL:HG22	1.51	0.76
1:D:741:HIS:CD2	1:D:744:ARG:H	2.03	0.75
2:G:1656:LYS:NZ	2:G:1682:THR:HG23	2.01	0.75
2:G:1699:LEU:H	2:G:1699:LEU:CD1	1.98	0.75
2:H:1440:LEU:HD11	2:H:1468:ARG:HD2	1.68	0.75
1:A:103:LEU:HD13	1:A:146:LEU:HD11	1.67	0.75
2:G:1620:ASN:HD22	2:G:1632:GLN:HE21	1.35	0.75
1:C:546:LEU:HD12	1:C:591:LEU:HD12	1.68	0.74
1:C:541:HIS:ND1	1:C:542:PRO:HD2	2.04	0.72
2:E:1287:LEU:HD12	2:E:1287:LEU:H	1.51	0.72
1:C:497:LEU:HD11	1:C:536:SER:HB3	1.71	0.72
2:F:1087:LEU:HD12	2:F:1087:LEU:H	1.52	0.72
1:B:363:ASP:OD1	1:B:364:ASP:N	2.23	0.72
1:C:412:ILE:O	1:C:413:SER:HB2	1.89	0.72
2:E:1222:VAL:HG21	2:E:1308:ILE:HD11	1.72	0.72
2:G:1699:LEU:HD12	2:G:1699:LEU:N	2.04	0.72
1:D:630:HIS:CE1	1:D:634:ASN:HD21	2.08	0.71
1:A:12:ILE:HD12	1:A:12:ILE:N	2.05	0.71
2:E:1240:LEU:HD11	2:E:1268:ARG:HD2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:637:GLN:OE1	2:H:1505:PRO:HA	1.90	0.71
1:C:519:HIS:O	1:C:522:ASP:HB3	1.90	0.71
1:A:38:LEU:HD13	1:A:54:MET:HE1	1.73	0.70
1:C:489:TYR:CZ	1:C:522:ASP:HB2	2.26	0.70
2:G:1650:LEU:HD23	2:G:1651:VAL:H	1.57	0.70
1:C:525:VAL:HB	1:C:531:ASN:ND2	2.07	0.70
2:F:1086:GLU:O	2:F:1090:ILE:HG13	1.91	0.70
1:B:377:ARG:HB3	1:B:388:GLU:HB2	1.73	0.70
2:G:1676:ILE:HG13	2:G:1677:ARG:H	1.56	0.69
1:A:103:LEU:HD13	1:A:146:LEU:CD1	2.21	0.69
2:G:1692:GLU:OE1	2:G:1696:LEU:HD11	1.92	0.69
1:B:370:TYR:HD2	1:B:373:VAL:CG2	2.06	0.69
2:G:1610:ASP:OD1	2:G:1654:BFD:HB3	1.94	0.68
1:C:489:TYR:N	1:C:489:TYR:CD1	2.55	0.68
1:B:344:ARG:NH2	1:B:374:ASP:OD2	2.26	0.68
2:H:1494:LYS:HD3	2:H:1501[B]:HIS:NE2	2.09	0.67
1:D:710:LEU:HD21	1:D:791:LEU:HD22	1.76	0.67
1:C:570:TYR:O	1:C:573:VAL:HG22	1.94	0.67
1:D:781:THR:HG23	1:D:784:GLU:H	1.60	0.67
2:F:1099:LEU:HD23	2:F:1118:TYR:CD1	2.29	0.67
2:G:1610:ASP:OD2	2:G:1612:GLN:HG2	1.95	0.66
2:G:1640:LEU:O	2:G:1640:LEU:HD23	1.95	0.66
2:G:1694:LYS:HA	2:G:1698:ALA:HB3	1.77	0.66
1:D:741:HIS:HD2	1:D:744:ARG:HB2	1.60	0.66
2:G:1677:ARG:HD2	2:G:1699:LEU:HD21	1.77	0.66
1:C:516:LYS:HG3	1:C:570:TYR:CE1	2.30	0.66
2:G:1690:ILE:N	2:G:1690:ILE:HD12	2.10	0.66
1:B:218:THR:O	1:B:222:ILE:HG13	1.96	0.66
2:G:1668:ARG:O	2:G:1671:VAL:HB	1.96	0.66
2:G:1604:GLU:H	2:G:1604:GLU:CD	1.99	0.66
2:H:1487:LEU:HD12	2:H:1487:LEU:H	1.60	0.66
2:G:1665:ILE:HD12	2:G:1668:ARG:HB2	1.78	0.66
2:G:1687:LEU:CA	2:G:1690:ILE:HD13	2.16	0.66
1:B:362:PHE:O	1:B:366:ARG:HG3	1.96	0.66
2:H:1499:LEU:HD23	2:H:1518:TYR:CD1	2.31	0.65
1:D:775:ILE:HG13	1:D:775:ILE:O	1.96	0.65
1:C:541:HIS:HD2	1:C:544:ARG:H	1.45	0.65
2:G:1611:ASP:HB3	2:G:1657:ILE:HG23	1.79	0.65
1:A:35:LYS:HD3	1:A:58:MET:HG2	1.79	0.65
1:C:478:PHE:CD2	1:D:621:LEU:HD23	2.32	0.64
2:G:1622:VAL:O	2:G:1626:GLU:HG2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:PRO:HD2	1:A:107:ASP:OD1	1.98	0.64
2:E:1286:GLU:O	2:E:1290:ILE:HG13	1.98	0.64
1:A:38:LEU:HD22	1:A:54:MET:HE1	1.80	0.64
1:B:235:LYS:HD3	1:B:258:MET:HG2	1.80	0.64
1:A:71:LEU:HB2	1:A:73:THR:CG2	2.28	0.64
2:G:1657:ILE:CG2	2:G:1658:PRO:HD2	2.27	0.64
1:C:471:LEU:HB2	1:C:473:THR:CG2	2.27	0.64
1:D:709:LYS:HB2	1:D:709:LYS:HZ2	1.60	0.64
1:A:46:GLN:HG2	1:A:48:TYR:OH	1.98	0.64
1:C:412:ILE:HG12	1:D:715:ARG:HH12	1.62	0.64
1:D:647:LYS:HB2	1:D:647:LYS:NZ	2.12	0.64
1:D:745:GLN:HB3	1:D:792:ASP:HA	1.78	0.64
1:C:516:LYS:HE2	1:C:520:LEU:HD21	1.78	0.63
2:E:1218:LEU:O	2:E:1222:VAL:HG23	1.98	0.63
1:C:522:ASP:O	1:C:527:ARG:NH2	2.31	0.63
2:F:1099:LEU:HD23	2:F:1118:TYR:CG	2.34	0.63
2:G:1660:MET:HE1	2:G:1664:GLU:HB3	1.80	0.63
1:A:17:LEU:HD23	1:A:18:THR:N	2.12	0.63
2:G:1682:THR:O	2:G:1703:ALA:HA	1.97	0.63
1:D:735:VAL:HG22	1:D:750:LEU:HG	1.81	0.63
2:H:1499:LEU:HD23	2:H:1518:TYR:CG	2.33	0.63
2:F:1040:LEU:HD11	2:F:1068:ARG:HD2	1.81	0.63
2:G:1633:ALA:HB1	2:G:1639:ALA:HB2	1.79	0.63
1:A:75:HIS:ND1	1:A:108:GLN:NE2	2.46	0.63
1:A:175:ILE:O	1:A:175:ILE:HG22	1.99	0.63
2:H:1486:GLU:O	2:H:1490:ILE:HG13	1.98	0.63
2:G:1655:MET:CE	2:G:1689:MET:HG2	2.28	0.62
2:G:1616:ARG:NH1	2:G:1634:ALA:HA	2.13	0.62
2:G:1650:LEU:HD23	2:G:1651:VAL:N	2.14	0.62
1:B:335:VAL:HG22	1:B:350:LEU:HG	1.81	0.62
2:G:1620:ASN:HD22	2:G:1632:GLN:HG3	1.65	0.62
1:D:706:TYR:N	1:D:706:TYR:CD1	2.66	0.62
2:G:1656:LYS:HZ3	2:G:1682:THR:HG23	1.62	0.62
1:B:364:ASP:OD1	1:B:364:ASP:C	2.38	0.62
1:B:381:THR:HG23	1:C:581:THR:CG2	2.27	0.62
1:C:412:ILE:CG1	1:D:715:ARG:HH12	2.12	0.61
1:C:489:TYR:CE2	1:C:522:ASP:HA	2.36	0.61
2:G:1660:MET:CE	2:G:1664:GLU:HB3	2.30	0.61
2:H:1418:LEU:O	2:H:1422:VAL:HG23	2.00	0.61
1:D:633:MET:CE	1:D:636:LEU:HD12	2.31	0.60
1:B:217:LEU:HD23	1:B:218:THR:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:GLN:HE21	1:B:345:GLN:HA	1.66	0.60
1:D:741:HIS:ND1	1:D:742:PRO:HD2	2.17	0.60
1:A:178:PHE:HD1	1:A:178:PHE:O	1.85	0.60
1:B:260:ILE:HG22	1:B:261:ASP:N	2.16	0.60
1:B:327:ARG:C	2:F:1037:LEU:HD12	2.21	0.60
1:C:575:ILE:HD11	1:C:578:PHE:CD2	2.36	0.60
1:A:141:HIS:CD2	1:A:144:ARG:H	2.07	0.59
1:A:168:ASN:HD22	1:A:168:ASN:N	1.99	0.59
1:A:12:ILE:O	1:A:13:SER:HB2	2.00	0.59
2:F:1018:LEU:O	2:F:1022:VAL:HG23	2.02	0.59
2:G:1650:LEU:HD22	2:G:1652:LEU:CD1	2.32	0.59
2:E:1299:LEU:HD23	2:E:1318:TYR:CD1	2.38	0.59
2:G:1679:ILE:HG23	2:G:1700:THR:HG23	1.82	0.59
1:B:379:GLU:HG3	1:C:580:ILE:O	2.01	0.59
2:G:1680:ILE:HG22	2:G:1681:MET:N	2.17	0.59
1:C:418:THR:O	1:C:422:ILE:HD13	2.02	0.59
1:D:665:GLU:HA	1:D:694:TYR:OH	2.01	0.59
1:A:78:PHE:HD2	1:B:221:LEU:HD22	1.66	0.58
1:C:558:ASP:OD1	1:C:558:ASP:O	2.21	0.58
2:H:1440:LEU:CD1	2:H:1468:ARG:HD2	2.33	0.58
1:C:541:HIS:CD2	1:C:544:ARG:H	2.22	0.58
1:C:497:LEU:CD1	1:C:536:SER:HB3	2.34	0.58
1:D:705:ALA:HB3	1:D:706:TYR:CE1	2.38	0.58
1:A:125:VAL:HB	1:A:131:ASN:ND2	2.18	0.58
1:C:412:ILE:HG12	1:D:715:ARG:NH1	2.18	0.58
1:C:441:GLY:HA3	2:G:1618:LEU:HD21	1.85	0.58
1:B:345:GLN:HB3	1:B:392:ASP:HA	1.84	0.58
2:G:1643:VAL:HA	2:G:1648:PRO:CD	2.34	0.58
1:A:73:THR:OG1	1:A:76:LEU:HB3	2.03	0.58
1:B:341:HIS:CD2	1:B:343:ASP:H	2.22	0.58
1:C:417:LEU:HD21	1:C:421:LEU:HD11	1.86	0.57
1:C:562:PHE:HA	1:C:565:ILE:HD13	1.84	0.57
2:F:1082:THR:O	2:F:1103:ALA:HA	2.04	0.57
1:A:24:LEU:HG	1:B:221:LEU:HD11	1.86	0.57
1:C:437:GLN:O	1:C:437:GLN:NE2	2.38	0.57
2:E:1314:ALA:O	2:E:1318:TYR:HD2	1.88	0.57
1:B:358:ASP:OD1	1:B:360:SER:HB3	2.04	0.57
2:F:1007:LEU:HB3	2:F:1051:VAL:HG22	1.85	0.57
1:A:78:PHE:CE2	1:B:221:LEU:HD22	2.40	0.57
1:C:575:ILE:HD11	1:C:578:PHE:HD2	1.70	0.57
2:G:1717:LYS:HE3	2:G:1718:TYR:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:ARG:O	1:C:454:MET:HG3	2.05	0.56
1:A:141:HIS:HD2	1:A:144:ARG:N	1.96	0.56
1:D:790:GLY:O	1:D:791:LEU:HD12	2.04	0.56
2:E:1240:LEU:CD1	2:E:1268:ARG:HD2	2.34	0.56
2:F:1055:MET:HE3	2:F:1089:MET:HB3	1.88	0.56
2:G:1643:VAL:HA	2:G:1648:PRO:HD3	1.88	0.56
1:C:537:LEU:N	1:C:537:LEU:HD12	2.20	0.56
2:F:1114:ALA:O	2:F:1118:TYR:HD2	1.88	0.56
1:B:249:ASP:O	1:B:253:GLU:HG3	2.06	0.56
1:A:72:LYS:HB3	1:A:104:SER:HB3	1.86	0.56
1:C:500:ILE:HD12	1:C:500:ILE:N	2.21	0.56
2:F:1040:LEU:CD1	2:F:1068:ARG:HD2	2.36	0.56
2:G:1604:GLU:CG	2:G:1720:PRO:HG2	2.36	0.56
1:C:508:GLN:HA	1:C:508:GLN:NE2	2.21	0.56
2:G:1690:ILE:HD12	2:G:1690:ILE:H	1.71	0.56
1:D:651:VAL:O	1:D:655:ILE:HG13	2.06	0.56
2:E:1266:LEU:O	2:E:1266:LEU:HD22	2.06	0.56
2:F:1052:LEU:HB3	2:F:1081:MET:HE1	1.88	0.56
2:G:1692:GLU:O	2:G:1696:LEU:HG	2.05	0.56
2:G:1636:GLY:HA3	2:G:1660:MET:HG2	1.88	0.55
1:C:437:GLN:CG	2:G:1704:LYS:HB2	2.36	0.55
2:E:1282:THR:O	2:E:1303:ALA:HA	2.06	0.55
2:F:1054:BFD:F1	2:F:1056:LYS:HB2	1.96	0.55
1:A:24:LEU:HD12	1:A:85:TRP:CZ3	2.42	0.55
1:C:471:LEU:HD23	1:C:500:ILE:HG23	1.89	0.55
1:D:654:MET:O	1:D:658:MET:HG3	2.06	0.55
2:G:1691:GLN:NE2	2:G:1691:GLN:HA	2.21	0.55
1:B:364:ASP:OD1	1:B:365:ILE:N	2.39	0.55
1:D:646:GLN:HG2	1:D:648:TYR:OH	2.05	0.55
1:B:331:ASN:HB3	1:B:352:PHE:HE1	1.71	0.55
1:C:514:MET:HG3	1:C:518:PHE:CZ	2.41	0.55
1:D:746:LEU:HD22	1:D:747:ILE:N	2.22	0.55
1:D:706:TYR:HE2	1:D:792:ASP:O	1.89	0.55
1:D:647:LYS:HB2	1:D:647:LYS:HZ2	1.72	0.55
1:D:771:GLU:HG3	1:D:772:ASP:H	1.72	0.55
2:E:1299:LEU:HD23	2:E:1318:TYR:CG	2.42	0.55
2:E:1312:ARG:O	2:E:1315:VAL:HG22	2.07	0.54
2:G:1620:ASN:ND2	2:G:1632:GLN:NE2	2.44	0.54
1:D:655:ILE:O	1:D:659:VAL:HG23	2.07	0.54
2:G:1620:ASN:HD22	2:G:1632:GLN:NE2	2.05	0.54
2:H:1455:MET:CE	2:H:1489:MET:HB3	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1691:GLN:HA	2:G:1691:GLN:HE21	1.73	0.54
1:D:665:GLU:HG2	1:D:694:TYR:OH	2.08	0.54
2:G:1604:GLU:HG3	2:G:1720:PRO:HG2	1.90	0.54
2:G:1657:ILE:HG22	2:G:1658:PRO:HD2	1.88	0.54
1:C:521:PHE:O	1:C:525:VAL:HG13	2.07	0.54
1:D:683:PHE:CD1	1:D:692:LEU:HB3	2.42	0.54
1:C:526:SER:OG	1:C:528:GLU:HG2	2.08	0.54
2:F:1121:LEU:N	2:F:1121:LEU:HD13	2.22	0.54
2:G:1605:LYS:HB3	2:G:1629:GLN:HB2	1.90	0.54
2:H:1443:VAL:HG21	2:H:1469:MET:CE	2.37	0.54
1:B:264:HIS:CD2	1:B:295:GLU:HG2	2.43	0.53
2:G:1680:ILE:CG2	2:G:1681:MET:N	2.71	0.53
2:G:1684:TYR:O	2:G:1686:GLU:N	2.41	0.53
1:A:37:GLN:HA	2:E:1305:PRO:HB3	1.89	0.53
1:D:741:HIS:HE2	1:D:743:ASP:HB2	1.74	0.53
1:D:744:ARG:NH2	1:D:774:ASP:OD2	2.42	0.53
2:G:1641:ASP:O	2:G:1645:LYS:HG2	2.08	0.53
2:G:1707:ASP:HB3	2:G:1710:GLU:CG	2.38	0.53
1:C:549:TYR:C	1:C:550:LEU:HD12	2.29	0.53
1:D:703:LEU:O	1:D:706:TYR:HD1	1.91	0.53
2:G:1715:VAL:HG23	2:G:1716:LYS:N	2.23	0.53
1:D:771:GLU:HG3	1:D:772:ASP:N	2.22	0.53
2:G:1655:MET:HE3	2:G:1689:MET:HG2	1.89	0.53
2:F:1052:LEU:HB3	2:F:1081:MET:CE	2.38	0.53
2:F:1055:MET:CE	2:F:1089:MET:HB3	2.39	0.53
2:G:1699:LEU:HD23	2:G:1718:TYR:CD2	2.43	0.53
2:H:1515:VAL:HG23	2:H:1516:LYS:N	2.24	0.53
1:A:141:HIS:CD2	1:A:143:ASP:H	2.27	0.53
1:B:377:ARG:HG3	1:B:379:GLU:OE2	2.09	0.53
1:C:520:LEU:HD11	1:C:565:ILE:HG12	1.91	0.53
1:C:544:ARG:NH2	1:C:574:ASP:HB3	2.24	0.53
1:D:627:HIS:ND1	1:D:685:TRP:HB3	2.23	0.53
2:F:1107:ASP:HB2	2:F:1110:GLU:HG2	1.91	0.53
2:H:1512:ARG:O	2:H:1515:VAL:HG22	2.09	0.53
1:A:108:GLN:OE1	1:A:108:GLN:HA	2.07	0.53
1:C:489:TYR:HD2	1:C:490:MET:HG2	1.73	0.53
1:C:560:SER:HA	1:C:563:ASP:OD2	2.09	0.53
2:F:1112:ARG:O	2:F:1115:VAL:HG22	2.09	0.53
2:H:1407:LEU:HB3	2:H:1451:VAL:HG22	1.90	0.52
1:B:277:ALA:O	1:B:281:LEU:HG	2.09	0.52
2:H:1454:BFD:F1	2:H:1456:LYS:HB2	1.99	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:515:ARG:HH11	1:C:515:ARG:CB	2.17	0.52
2:E:1251:VAL:CG1	2:E:1269:MET:HE1	2.26	0.52
2:G:1616:ARG:NH1	2:G:1634:ALA:CB	2.72	0.52
1:B:386:LEU:HD13	1:B:386:LEU:C	2.30	0.52
1:C:472:LYS:HB3	1:C:504:SER:HB2	1.91	0.52
1:C:501:LYS:HD2	1:C:503:LEU:HD21	1.91	0.52
1:D:749:TYR:C	1:D:750:LEU:HD12	2.29	0.52
1:C:566:ARG:HD2	1:C:578:PHE:CD1	2.45	0.52
1:D:633:MET:HE2	1:D:636:LEU:HD12	1.90	0.52
1:A:24:LEU:HD12	1:A:85:TRP:CE3	2.45	0.52
1:C:446:GLN:HA	1:C:448:TYR:CE2	2.45	0.52
1:C:489:TYR:CZ	1:C:522:ASP:HA	2.45	0.52
2:F:1115:VAL:HG23	2:F:1116:LYS:N	2.25	0.52
2:H:1521:LEU:N	2:H:1521:LEU:HD13	2.24	0.52
1:A:12:ILE:HG13	1:B:315:ARG:CZ	2.40	0.52
1:B:212:ILE:HD12	1:B:212:ILE:N	2.24	0.52
1:B:381:THR:CG2	1:C:581:THR:HG23	2.31	0.52
1:C:437:GLN:HG2	2:G:1704:LYS:HB2	1.91	0.51
1:D:741:HIS:NE2	1:D:743:ASP:HB2	2.25	0.51
2:E:1321:LEU:HD13	2:E:1321:LEU:N	2.25	0.51
1:C:500:ILE:HD12	1:C:500:ILE:H	1.75	0.51
1:A:127:ARG:HH11	1:A:127:ARG:CG	2.20	0.51
1:C:473:THR:OG1	1:C:476:LEU:HB3	2.11	0.51
2:E:1234:ALA:H	2:E:1238:GLN:NE2	2.08	0.51
1:C:580:ILE:O	1:C:580:ILE:HG12	2.09	0.51
2:G:1655:MET:HE2	2:G:1689:MET:HG2	1.92	0.51
1:B:234:ASN:O	1:B:237:GLN:HB3	2.10	0.51
1:C:433:MET:HE1	1:D:659:VAL:HG13	1.93	0.51
1:C:549:TYR:N	1:C:549:TYR:CD2	2.79	0.51
2:F:1070:LYS:HD3	2:F:1076:ILE:HG22	1.93	0.51
2:G:1604:GLU:HB3	2:G:1720:PRO:HG2	1.92	0.51
2:G:1668:ARG:H	2:G:1668:ARG:HD2	1.75	0.51
2:H:1455:MET:HE2	2:H:1489:MET:HB3	1.93	0.51
2:G:1652:LEU:CD1	2:G:1652:LEU:N	2.73	0.51
1:A:190:GLY:O	1:A:191:LEU:HD12	2.11	0.51
1:B:211:ASN:OD1	1:B:212:ILE:N	2.43	0.51
1:B:338:GLN:NE2	1:B:349:TYR:OH	2.44	0.51
1:D:717:LEU:HD13	1:D:750:LEU:CD2	2.41	0.51
2:E:1315:VAL:HG23	2:E:1316:LYS:N	2.26	0.51
2:G:1616:ARG:HG2	2:G:1632:GLN:OE1	2.11	0.51
2:G:1670:LYS:HA	2:G:1673:ASP:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:478:PHE:CE2	1:D:621:LEU:HD23	2.45	0.51
2:E:1254:BFD:F1	2:E:1256:LYS:HB2	2.01	0.51
2:E:1307:ASP:HB2	2:E:1310:GLU:HG2	1.92	0.51
1:B:212:ILE:HD12	1:B:212:ILE:H	1.76	0.50
1:C:412:ILE:O	1:C:413:SER:CB	2.58	0.50
2:G:1642:ILE:O	2:G:1646:GLU:HB3	2.11	0.50
1:A:38:LEU:HD13	1:A:54:MET:CE	2.40	0.50
1:B:328:GLU:HA	2:F:1037:LEU:HB2	1.93	0.50
1:C:420:GLU:OE2	1:C:420:GLU:HA	2.11	0.50
1:C:426:GLY:HA2	1:C:429:ARG:NH2	2.26	0.50
1:C:520:LEU:CD1	1:C:565:ILE:HG12	2.41	0.50
1:A:178:PHE:O	1:A:178:PHE:CD1	2.64	0.50
1:C:516:LYS:HG3	1:C:570:TYR:CZ	2.46	0.50
1:B:288:HIS:HD2	1:B:322:ASP:OD2	1.94	0.50
1:D:683:PHE:CB	1:D:692:LEU:HD23	2.41	0.50
2:F:1080:ILE:O	2:F:1101:HIS:HA	2.11	0.50
2:H:1494:LYS:HD3	2:H:1501[B]:HIS:CE1	2.46	0.50
2:H:1507:ASP:HB2	2:H:1510:GLU:HG2	1.93	0.50
1:C:449:ASP:O	1:C:453:GLU:HG3	2.12	0.50
1:A:191:LEU:HD12	1:A:191:LEU:N	2.27	0.50
1:C:482:THR:HA	1:C:485:TRP:CE3	2.46	0.50
1:C:489:TYR:CE2	1:C:490:MET:HG2	2.47	0.50
1:C:510:LEU:HD21	1:C:591:LEU:CD1	2.42	0.50
2:E:1204:GLU:HG2	2:E:1249:ASP:OD1	2.12	0.50
2:G:1699:LEU:HD23	2:G:1718:TYR:CE2	2.47	0.50
1:C:420:GLU:O	1:C:424:LEU:HG	2.12	0.50
2:G:1620:ASN:HD22	2:G:1632:GLN:CG	2.25	0.50
2:G:1717:LYS:HE3	2:G:1718:TYR:CZ	2.47	0.50
1:A:177:ARG:HB3	1:A:188:GLU:HB2	1.94	0.49
2:G:1663:ILE:HD13	2:G:1663:ILE:O	2.12	0.49
1:C:480:PHE:CE2	1:C:514:MET:HG2	2.48	0.49
1:C:486:LYS:HB2	1:C:488:HIS:HE1	1.77	0.49
1:C:541:HIS:CG	1:C:542:PRO:HD2	2.47	0.49
2:E:1280:ILE:O	2:E:1301:HIS:HA	2.12	0.49
1:A:37:GLN:OE1	2:E:1305:PRO:HA	2.12	0.49
1:A:72:LYS:C	1:A:74:PRO:HD3	2.32	0.49
2:G:1612:GLN:HA	2:G:1612:GLN:HE21	1.77	0.49
1:D:740:ASP:OD1	1:D:740:ASP:O	2.30	0.49
1:A:55:ILE:O	1:A:59:VAL:HG23	2.13	0.49
1:D:678:PHE:CE1	1:D:682:THR:HG21	2.48	0.49
2:G:1700:THR:OG1	2:G:1701:HIS:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:HIS:ND1	2:E:1283:ALA:HB3	2.27	0.49
1:C:578:PHE:HD1	1:C:578:PHE:O	1.95	0.49
2:G:1676:ILE:HG13	2:G:1677:ARG:N	2.25	0.49
1:A:17:LEU:CG	1:A:21:LEU:HD11	2.38	0.48
1:B:272:LYS:HB3	1:B:304:SER:HB3	1.94	0.48
1:B:372:ASP:OD2	1:B:372:ASP:C	2.50	0.48
2:G:1670:LYS:HE3	2:G:1674:GLU:O	2.12	0.48
1:A:17:LEU:HG	1:A:21:LEU:CD1	2.39	0.48
1:D:617:LEU:C	1:D:617:LEU:HD23	2.34	0.48
2:G:1618:LEU:O	2:G:1622:VAL:HG23	2.13	0.48
2:G:1652:LEU:N	2:G:1652:LEU:HD12	2.27	0.48
2:G:1711:ILE:C	2:G:1713:ASP:H	2.15	0.48
1:C:417:LEU:CD2	1:C:421:LEU:HD11	2.43	0.48
1:C:424:LEU:HD12	1:D:621:LEU:HD22	1.96	0.48
1:D:647:LYS:HG2	1:D:650:ARG:CB	2.43	0.48
1:B:350:LEU:HB2	1:B:387:ILE:HB	1.93	0.48
2:H:1482:THR:O	2:H:1503:ALA:HA	2.13	0.48
1:D:744:ARG:HE	1:D:776:MET:HE3	1.78	0.48
2:G:1715:VAL:HG23	2:G:1716:LYS:H	1.78	0.48
1:B:349:TYR:C	1:B:350:LEU:HD12	2.34	0.48
2:E:1211:ASP:HB3	2:E:1258:PRO:HD2	1.96	0.48
1:D:634:ASN:O	1:D:637:GLN:HB3	2.13	0.48
2:E:1228:TYR:CE1	2:E:1319:LEU:HD23	2.49	0.48
2:G:1690:ILE:H	2:G:1690:ILE:CD1	2.27	0.48
1:A:12:ILE:N	1:A:12:ILE:CD1	2.75	0.48
1:D:612:ILE:HG13	1:D:612:ILE:O	2.14	0.48
2:H:1443:VAL:HG21	2:H:1469:MET:HE3	1.95	0.48
2:G:1668:ARG:HD2	2:G:1668:ARG:N	2.29	0.47
2:G:1700:THR:O	2:G:1701:HIS:HB3	2.14	0.47
1:A:101:LYS:HD3	1:A:139:THR:HB	1.95	0.47
1:C:469:SER:HB3	1:D:622:ILE:CG2	2.43	0.47
2:G:1684:TYR:O	2:G:1685:GLY:C	2.52	0.47
1:A:93:GLU:HB2	1:A:132:HIS:NE2	2.28	0.47
1:D:781:THR:OG1	1:D:782:SER:N	2.44	0.47
2:H:1491:GLN:O	2:H:1495:GLU:HG3	2.14	0.47
1:A:20:GLU:HG3	1:A:24:LEU:HD23	1.96	0.47
2:G:1640:LEU:HD12	2:G:1668:ARG:HG2	1.97	0.47
1:C:489:TYR:CD2	1:C:522:ASP:HA	2.49	0.47
1:D:738:GLN:O	1:D:746:LEU:HD23	2.15	0.47
1:B:250:ARG:HE	1:B:254:MET:HE3	1.80	0.47
2:H:1428:TYR:CE1	2:H:1519:LEU:HD23	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1011:ASP:HB3	2:F:1058:PRO:HD2	1.97	0.47
2:G:1624:ASN:HA	2:G:1628:TYR:O	2.14	0.47
1:A:21:LEU:CD2	1:B:221:LEU:HB2	2.45	0.47
1:C:529:SER:CB	1:C:555:ALA:HB3	2.45	0.47
1:D:721:PHE:O	1:D:725:VAL:HG22	2.15	0.47
2:E:1311:ILE:O	2:E:1315:VAL:HG13	2.15	0.47
1:A:103:LEU:HD22	1:A:146:LEU:HD12	1.97	0.46
1:C:418:THR:HG22	1:D:674:PRO:HB2	1.96	0.46
1:C:489:TYR:OH	1:C:522:ASP:HB2	2.15	0.46
2:G:1604:GLU:HB2	2:G:1649:ASP:OD1	2.15	0.46
2:G:1667:LYS:O	2:G:1671:VAL:HG23	2.15	0.46
1:B:328:GLU:CD	1:B:328:GLU:O	2.54	0.46
2:F:1087:LEU:HD12	2:F:1087:LEU:N	2.27	0.46
2:H:1475:ASN:N	2:H:1475:ASN:HD22	2.13	0.46
1:B:283:PHE:CD1	1:B:292:LEU:HB3	2.50	0.46
1:B:331:ASN:HB3	1:B:352:PHE:CE1	2.49	0.46
2:G:1653:LEU:HG	2:G:1654:BFD:O	2.16	0.46
2:H:1411:ASP:HB3	2:H:1458:PRO:HD2	1.97	0.46
1:A:141:HIS:CD2	1:A:144:ARG:HG2	2.51	0.46
1:C:424:LEU:CD1	1:D:621:LEU:HD22	2.46	0.46
2:E:1231:PHE:CE1	2:E:1246:GLU:HG3	2.49	0.46
2:G:1680:ILE:HD11	2:G:1693:SER:HB2	1.96	0.46
1:A:43:LEU:HD23	1:A:51:VAL:HG21	1.97	0.46
1:D:650:ARG:O	1:D:654:MET:HG3	2.16	0.46
2:G:1620:ASN:ND2	2:G:1632:GLN:HG3	2.28	0.46
1:D:703:LEU:HD11	1:D:739:THR:HG22	1.98	0.46
1:D:777:ARG:HE	1:D:779:GLU:CG	2.29	0.46
2:G:1604:GLU:CB	2:G:1720:PRO:HG2	2.46	0.46
1:C:489:TYR:CE1	1:C:522:ASP:HB2	2.51	0.46
1:C:508:GLN:HE21	1:C:508:GLN:CA	2.29	0.46
2:E:1301:HIS:C	2:E:1301:HIS:CD2	2.88	0.46
2:H:1491:GLN:HA	2:H:1491:GLN:NE2	2.31	0.46
1:D:694:TYR:CD1	1:D:694:TYR:C	2.89	0.45
1:D:762:PHE:O	1:D:766:ARG:HG3	2.16	0.45
1:C:443:LEU:HD22	1:C:443:LEU:O	2.15	0.45
2:E:1275:ASN:HD22	2:E:1275:ASN:N	2.13	0.45
1:A:141:HIS:CG	1:A:142:PRO:HD2	2.51	0.45
1:C:443:LEU:HD13	1:D:652:PHE:CZ	2.52	0.45
2:H:1428:TYR:OH	2:H:1516:LYS:HG3	2.17	0.45
1:C:508:GLN:HA	1:C:508:GLN:HE21	1.81	0.45
1:D:744:ARG:NH1	1:D:744:ARG:HG2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1646:GLU:O	2:G:1647:ARG:C	2.55	0.45
2:H:1452:LEU:HB3	2:H:1481:MET:CE	2.47	0.45
1:A:14:ASP:OD2	1:A:16:ALA:HB3	2.17	0.45
1:A:170:TYR:O	1:A:173:VAL:HG22	2.16	0.45
1:B:237:GLN:HE22	2:F:1106:PHE:H	1.63	0.45
1:B:308:GLN:NE2	1:B:308:GLN:HA	2.31	0.45
1:B:390:GLY:C	1:B:391:LEU:HD12	2.37	0.45
1:C:417:LEU:O	1:C:421:LEU:HG	2.17	0.45
1:C:489:TYR:CZ	1:C:522:ASP:CB	2.99	0.45
1:C:489:TYR:HB2	1:C:525:VAL:HG21	1.98	0.45
1:D:780:ILE:HG12	1:D:780:ILE:O	2.17	0.45
2:E:1249:ASP:HB3	2:E:1319:LEU:HD11	1.99	0.45
2:G:1715:VAL:O	2:G:1718:TYR:N	2.46	0.45
2:G:1719:LEU:HD23	2:G:1720:PRO:HD2	1.99	0.45
1:A:34:ASN:O	1:A:37:GLN:HB3	2.17	0.45
1:A:75:HIS:HD2	1:B:218:THR:HG21	1.82	0.45
2:E:1270:LYS:HD3	2:E:1276:ILE:HG22	1.99	0.45
2:E:1319:LEU:O	2:E:1320:PRO:O	2.35	0.45
1:A:88:HIS:HD2	1:A:122:ASP:OD1	2.00	0.45
1:B:235:LYS:CD	1:B:258:MET:HG2	2.46	0.45
1:C:442:ASN:ND2	1:C:447:LYS:HE2	2.32	0.45
1:D:729:SER:CB	1:D:755:ALA:HB3	2.47	0.45
2:F:1053:LEU:HD11	2:F:1065:ILE:HD13	1.99	0.45
2:G:1637:LEU:C	2:G:1639:ALA:N	2.69	0.45
1:B:341:HIS:HA	1:B:342:PRO:HD3	1.71	0.44
1:B:356:PHE:CB	1:B:359:PRO:HG3	2.47	0.44
1:D:777:ARG:HE	1:D:779:GLU:HG3	1.83	0.44
1:A:129:SER:CB	1:A:155:ALA:HB3	2.47	0.44
1:B:221:LEU:O	1:B:221:LEU:HG	2.16	0.44
1:A:168:ASN:N	1:A:168:ASN:ND2	2.65	0.44
1:C:471:LEU:O	1:C:472:LYS:HB2	2.16	0.44
1:C:510:LEU:HD21	1:C:591:LEU:HD11	1.99	0.44
2:F:1023:PHE:O	2:F:1028:TYR:HB2	2.18	0.44
2:G:1657:ILE:HG23	2:G:1658:PRO:HD2	1.99	0.44
1:A:12:ILE:O	1:A:13:SER:CB	2.66	0.44
1:A:91:THR:O	1:A:132:HIS:HD2	2.01	0.44
1:D:737:LEU:HG	1:D:748:LEU:HD12	2.00	0.44
1:A:127:ARG:HG3	1:A:127:ARG:NH1	2.25	0.44
1:A:129:SER:OG	1:A:155:ALA:HB3	2.17	0.44
1:B:370:TYR:CD2	1:B:373:VAL:HG22	2.42	0.44
1:C:437:GLN:HG3	2:G:1704:LYS:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ILE:HG22	1:A:148:LEU:N	2.33	0.44
2:E:1252:LEU:N	2:E:1252:LEU:HD12	2.33	0.44
2:F:1115:VAL:O	2:F:1119:LEU:HB2	2.18	0.44
1:C:546:LEU:HD13	1:C:546:LEU:C	2.38	0.44
1:D:709:LYS:NZ	1:D:709:LYS:CB	2.74	0.44
2:G:1607:LEU:HD12	2:G:1608:ILE:N	2.33	0.44
1:A:135:VAL:HG22	1:A:150:LEU:HG	2.00	0.44
1:C:500:ILE:H	1:C:500:ILE:CD1	2.31	0.44
2:E:1300:THR:OG1	2:E:1301:HIS:N	2.46	0.44
1:C:510:LEU:CD2	1:C:591:LEU:HD11	2.48	0.44
1:D:781:THR:CG2	1:D:784:GLU:HB2	2.48	0.44
2:G:1636:GLY:O	2:G:1640:LEU:N	2.45	0.44
1:A:127:ARG:CG	1:A:127:ARG:NH1	2.79	0.43
1:C:570:TYR:HB3	1:C:573:VAL:CG2	2.47	0.43
2:G:1677:ARG:HB3	2:G:1699:LEU:HD21	2.00	0.43
1:A:121:PHE:O	1:A:125:VAL:HG22	2.19	0.43
1:B:314:MET:HE3	1:B:314:MET:HA	1.98	0.43
1:C:478:PHE:CE2	1:D:621:LEU:CD2	3.00	0.43
1:C:514:MET:HE3	1:C:548:LEU:HD13	2.00	0.43
2:E:1275:ASN:N	2:E:1275:ASN:ND2	2.66	0.43
2:G:1663:ILE:CG2	2:G:1664:GLU:N	2.82	0.43
2:H:1511:ILE:O	2:H:1515:VAL:HG13	2.18	0.43
1:B:379:GLU:HB2	1:C:581:THR:HG22	1.99	0.43
1:C:545:GLN:HB2	1:C:592:ASP:CB	2.43	0.43
2:F:1047:ARG:CZ	2:F:1073:ASP:HB2	2.49	0.43
2:H:1411:ASP:HB3	2:H:1457:ILE:HG23	2.00	0.43
1:D:701:LYS:HE2	1:D:739:THR:HB	2.01	0.43
1:D:717:LEU:HD13	1:D:750:LEU:HD22	2.01	0.43
1:D:771:GLU:CG	1:D:772:ASP:H	2.29	0.43
2:E:1276:ILE:HG23	2:E:1276:ILE:O	2.18	0.43
1:C:515:ARG:CB	1:C:515:ARG:NH1	2.81	0.43
2:F:1080:ILE:HD13	2:F:1093:SER:OG	2.18	0.43
2:G:1620:ASN:C	2:G:1622:VAL:H	2.22	0.43
1:D:741:HIS:CD2	1:D:744:ARG:N	2.80	0.43
1:B:281:LEU:HD23	1:B:294:TYR:OH	2.18	0.43
1:C:490:MET:HB3	1:C:531:ASN:HB2	2.00	0.43
1:C:514:MET:CG	1:C:518:PHE:CZ	3.02	0.43
1:A:75:HIS:CE1	1:A:108:GLN:HE22	2.34	0.42
1:C:468:LEU:HD21	1:C:477:ALA:HA	2.00	0.42
1:C:527:ARG:N	1:C:527:ARG:HD2	2.34	0.42
1:B:272:LYS:HE2	1:B:304:SER:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:448:TYR:N	1:C:448:TYR:CD2	2.84	0.42
1:C:483:PHE:HD1	1:C:484:ASN:HD22	1.65	0.42
1:D:625:LEU:HA	1:D:625:LEU:HD23	1.79	0.42
1:D:633:MET:HG3	2:H:1505:PRO:HD3	2.00	0.42
2:F:1066:LEU:O	2:F:1066:LEU:HD22	2.19	0.42
2:G:1693:SER:O	2:G:1698:ALA:HB2	2.19	0.42
2:H:1480:ILE:HD13	2:H:1493:SER:OG	2.19	0.42
1:A:113:LEU:O	1:A:116:LYS:HB3	2.19	0.42
1:B:326:SER:OG	1:B:329:SER:HB3	2.20	0.42
2:F:1100:THR:OG1	2:F:1101:HIS:N	2.50	0.42
2:G:1637:LEU:C	2:G:1639:ALA:H	2.23	0.42
2:H:1507:ASP:C	2:H:1509:ASP:N	2.72	0.42
1:B:320:LEU:HD23	1:B:320:LEU:HA	1.85	0.42
1:C:477:ALA:O	1:C:481:LEU:HG	2.19	0.42
2:H:1475:ASN:N	2:H:1475:ASN:ND2	2.67	0.42
1:C:486:LYS:HB2	1:C:488:HIS:CE1	2.54	0.42
2:F:1007:LEU:HD12	2:F:1008:ILE:N	2.33	0.42
2:F:1107:ASP:C	2:F:1109:ASP:N	2.71	0.42
1:C:514:MET:HA	1:C:517:LEU:HD12	2.01	0.42
2:F:1111:ILE:CG2	2:F:1112:ARG:N	2.82	0.42
2:G:1616:ARG:NH1	2:G:1634:ALA:CA	2.81	0.42
2:H:1407:LEU:HD12	2:H:1408:ILE:N	2.35	0.42
2:H:1467:LYS:HE3	2:H:1467:LYS:HB2	1.88	0.42
1:A:103:LEU:HD13	1:A:146:LEU:HD12	2.00	0.42
1:A:137:LEU:HG	1:A:148:LEU:CD1	2.50	0.42
2:G:1683:ALA:O	2:G:1685:GLY:N	2.52	0.42
2:G:1700:THR:HG23	2:G:1701:HIS:N	2.35	0.42
2:H:1419:LEU:O	2:H:1422:VAL:HB	2.20	0.42
1:C:423:HIS:NE2	1:C:427:HIS:CE1	2.88	0.42
2:H:1494:LYS:HD2	2:H:1494:LYS:HA	1.86	0.42
2:H:1514:ALA:O	2:H:1518:TYR:HD2	2.02	0.42
1:C:480:PHE:HE2	1:C:514:MET:HG2	1.83	0.42
1:C:489:TYR:CZ	1:C:522:ASP:CA	3.02	0.42
1:C:578:PHE:CD1	1:C:578:PHE:O	2.72	0.42
1:D:710:LEU:HD21	1:D:791:LEU:CD2	2.48	0.42
2:F:1049:ASP:O	2:F:1077:ARG:HD2	2.20	0.42
2:G:1660:MET:HE2	2:G:1661:ASP:O	2.20	0.42
2:G:1687:LEU:HD12	2:G:1690:ILE:HB	2.02	0.42
1:D:773:VAL:CG1	1:D:791:LEU:HD11	2.42	0.41
2:G:1620:ASN:CG	2:G:1632:GLN:HE21	2.19	0.41
2:G:1654:BFD:CG	2:G:1655:MET:H	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1663:ILE:HG23	2:G:1664:GLU:N	2.35	0.41
2:H:1519:LEU:O	2:H:1520:PRO:O	2.37	0.41
1:A:29:ARG:NH1	1:B:265:GLU:OE2	2.53	0.41
1:D:731:ASN:HB3	1:D:752:PHE:HE1	1.85	0.41
2:E:1315:VAL:O	2:E:1319:LEU:HB2	2.19	0.41
2:F:1077:ARG:HG2	2:F:1077:ARG:HH11	1.85	0.41
2:G:1640:LEU:HD23	2:G:1640:LEU:C	2.41	0.41
2:H:1452:LEU:N	2:H:1452:LEU:HD12	2.35	0.41
1:B:244:SER:C	1:B:246:GLN:H	2.24	0.41
1:B:306:TYR:OH	1:B:345:GLN:HG2	2.20	0.41
2:G:1699:LEU:HB3	2:G:1718:TYR:CE2	2.55	0.41
1:D:665:GLU:HA	1:D:694:TYR:HH	1.82	0.41
2:G:1691:GLN:NE2	2:G:1691:GLN:CA	2.83	0.41
2:H:1404:GLU:HG2	2:H:1449:ASP:OD1	2.19	0.41
1:A:137:LEU:HG	1:A:148:LEU:HD12	2.01	0.41
2:F:1070:LYS:HD3	2:F:1076:ILE:CG2	2.50	0.41
2:G:1609:VAL:HG22	2:G:1633:ALA:HB3	2.03	0.41
2:G:1646:GLU:O	2:G:1646:GLU:OE1	2.38	0.41
2:H:1515:VAL:O	2:H:1519:LEU:HB2	2.21	0.41
1:B:242:ASN:HD22	1:B:250:ARG:CG	2.34	0.41
1:B:263:LYS:HG3	2:E:1284:TYR:CE2	2.56	0.41
1:C:508:GLN:NE2	1:C:508:GLN:CA	2.83	0.41
1:A:162:PHE:CD1	1:A:178:PHE:HZ	2.39	0.41
1:B:230:HIS:CD2	2:F:1083:ALA:HB3	2.56	0.41
1:B:345:GLN:HA	1:B:345:GLN:NE2	2.34	0.41
1:C:417:LEU:HD23	1:C:418:THR:N	2.35	0.41
1:C:565:ILE:H	1:C:565:ILE:CD1	2.03	0.41
1:D:618:THR:O	1:D:622:ILE:HG13	2.20	0.41
2:E:1247:ARG:CZ	2:E:1273:ASP:HB2	2.51	0.41
2:G:1650:LEU:HD22	2:G:1652:LEU:HD12	2.01	0.41
2:G:1658:PRO:O	2:G:1660:MET:N	2.44	0.41
2:G:1699:LEU:O	2:G:1700:THR:HB	2.19	0.41
2:H:1470:LYS:HD3	2:H:1476:ILE:HG22	2.03	0.41
1:A:37:GLN:CA	2:E:1305:PRO:HB3	2.49	0.41
1:B:337:LEU:HD13	1:B:348:LEU:CD1	2.51	0.41
1:C:474:PRO:HB2	1:D:618:THR:HG22	2.03	0.41
1:A:37:GLN:HA	2:E:1305:PRO:CB	2.49	0.41
1:C:424:LEU:N	1:C:424:LEU:HD23	2.36	0.41
1:C:535:VAL:HG22	1:C:550:LEU:HG	2.03	0.41
1:C:538:GLN:OE1	1:C:547:ILE:HD12	2.20	0.41
1:D:716:LYS:HD3	1:D:716:LYS:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:737:LEU:HG	1:D:748:LEU:CD1	2.51	0.41
2:G:1646:GLU:O	2:G:1646:GLU:CD	2.58	0.41
2:G:1668:ARG:O	2:G:1669:MET:C	2.59	0.41
2:H:1443:VAL:HG21	2:H:1469:MET:HE2	2.03	0.41
2:H:1500:THR:OG1	2:H:1501[B]:HIS:N	2.53	0.41
2:H:1507:ASP:O	2:H:1509:ASP:N	2.53	0.41
1:A:46:GLN:HG2	1:A:48:TYR:CZ	2.55	0.41
1:A:50:ARG:O	1:A:54:MET:HG3	2.21	0.41
2:F:1043:VAL:HG21	2:F:1069:MET:CE	2.51	0.41
2:G:1650:LEU:HD22	2:G:1652:LEU:HD11	2.03	0.41
2:G:1664:GLU:HA	2:G:1667:LYS:HE3	2.02	0.41
1:A:152:PHE:HB3	1:A:185:CYS:HB3	2.02	0.40
1:D:744:ARG:HG2	1:D:744:ARG:HH11	1.86	0.40
2:G:1711:ILE:C	2:G:1713:ASP:N	2.74	0.40
2:H:1466:LEU:HD22	2:H:1466:LEU:O	2.20	0.40
1:B:312:LYS:HG2	1:B:370:TYR:OH	2.22	0.40
1:D:716:LYS:HG3	1:D:770:TYR:CE1	2.56	0.40
2:G:1623:PHE:HZ	2:G:1711:ILE:HG23	1.86	0.40
1:D:770:TYR:O	1:D:773:VAL:HG22	2.21	0.40
1:B:313:LEU:HD22	1:B:373:VAL:HG11	2.04	0.40
1:B:341:HIS:HD2	1:B:344:ARG:H	1.69	0.40
1:B:352:PHE:CG	1:B:353:HIS:N	2.89	0.40
1:D:647:LYS:HG2	1:D:650:ARG:HB2	2.02	0.40
1:D:706:TYR:CE2	1:D:792:ASP:O	2.72	0.40
2:E:1263:ILE:HD13	2:E:1263:ILE:HA	1.93	0.40
2:G:1623:PHE:CE1	2:G:1715:VAL:HG21	2.56	0.40
2:H:1499:LEU:CD1	2:H:1499:LEU:H	2.34	0.40
1:A:14:ASP:OD1	1:A:15:THR:N	2.54	0.40
1:B:289:TYR:CE2	1:B:327:ARG:HD3	2.57	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	179/192 (93%)	165 (92%)	12 (7%)	2 (1%)	14 42
1	B	180/192 (94%)	166 (92%)	13 (7%)	1 (1%)	25 55
1	C	179/192 (93%)	165 (92%)	12 (7%)	2 (1%)	14 42
1	D	180/192 (94%)	168 (93%)	11 (6%)	1 (1%)	25 55
2	E	116/124 (94%)	100 (86%)	15 (13%)	1 (1%)	17 47
2	F	116/124 (94%)	99 (85%)	14 (12%)	3 (3%)	5 22
2	G	116/124 (94%)	84 (72%)	20 (17%)	12 (10%)	0 2
2	H	117/124 (94%)	100 (86%)	14 (12%)	3 (3%)	5 22
All	All	1183/1264 (94%)	1047 (88%)	111 (9%)	25 (2%)	7 26

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	1320	PRO
2	F	1120	PRO
2	G	1684	TYR
2	G	1700	THR
2	H	1520	PRO
1	A	171	GLU
1	C	413	SER
2	G	1621	GLU
2	G	1646	GLU
2	G	1685	GLY
1	B	371	GLU
1	C	571	GLU
1	D	771	GLU
2	G	1701	HIS
2	G	1714	ALA
1	A	13	SER
2	F	1045	LYS
2	G	1659	GLY
2	G	1669	MET
2	G	1705	PRO
2	H	1518	TYR
2	H	1517	LYS
2	F	1117	LYS
2	G	1720	PRO
2	G	1708	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	166/177 (94%)	155 (93%)	11 (7%)	16	43
1	B	167/177 (94%)	152 (91%)	15 (9%)	9	30
1	C	166/177 (94%)	149 (90%)	17 (10%)	7	24
1	D	167/177 (94%)	151 (90%)	16 (10%)	8	27
2	E	104/109 (95%)	98 (94%)	6 (6%)	20	48
2	F	104/109 (95%)	99 (95%)	5 (5%)	25	55
2	G	104/109 (95%)	97 (93%)	7 (7%)	16	43
2	H	105/109 (96%)	97 (92%)	8 (8%)	13	38
All	All	1083/1144 (95%)	998 (92%)	85 (8%)	12	37

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	43	LEU
1	A	49	ASP
1	A	50	ARG
1	A	66	SER
1	A	93	GLU
1	A	116	LYS
1	A	145	GLN
1	A	151	ASP
1	A	166	ARG
1	A	186	LEU
1	B	212	ILE
1	B	213	SER
1	B	217	LEU
1	B	219	ASN
1	B	221	LEU
1	B	260	ILE
1	B	290	MET
1	B	328	GLU

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Mol	Chain	Res	Type
1	B	329	SER
1	B	336	SER
1	B	345	GLN
1	B	346	LEU
1	B	360	SER
1	B	364	ASP
1	B	392	ASP
1	C	425	LEU
1	C	437	GLN
1	C	443	LEU
1	C	445	LEU
1	C	489	TYR
1	C	490	MET
1	C	497	LEU
1	C	515	ARG
1	C	526	SER
1	C	546	LEU
1	C	548	LEU
1	C	551	ASP
1	C	564	ASP
1	C	566	ARG
1	C	580	ILE
1	C	582	SER
1	C	586	LEU
1	D	614	ASP
1	D	620	GLU
1	D	633	MET
1	D	638	LEU
1	D	647	LYS
1	D	656	GLU
1	D	682	THR
1	D	690	MET
1	D	691	THR
1	D	706	TYR
1	D	709	LYS
1	D	723	GLN
1	D	726	SER
1	D	746	LEU
1	D	768	ASN
1	D	780	ILE
2	E	1265	ILE
2	E	1266	LEU

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Mol	Chain	Res	Type
2	E	1292	GLU
2	E	1301	HIS
2	E	1311	ILE
2	E	1321	LEU
2	F	1065	ILE
2	F	1066	LEU
2	F	1092	GLU
2	F	1111	ILE
2	F	1121	LEU
2	G	1604	GLU
2	G	1605	LYS
2	G	1612	GLN
2	G	1650	LEU
2	G	1663	ILE
2	G	1669	MET
2	G	1711	ILE
2	H	1465	ILE
2	H	1466	LEU
2	H	1492	GLU
2	H	1501[A]	HIS
2	H	1501[B]	HIS
2	H	1511	ILE
2	H	1516	LYS
2	H	1521	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	34	ASN
1	A	88	HIS
1	A	108	GLN
1	A	132	HIS
1	A	141	HIS
1	A	168	ASN
1	B	219	ASN
1	B	223	HIS
1	B	227	HIS
1	B	230	HIS
1	B	237	GLN
1	B	242	ASN
1	B	264	HIS

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Mol	Chain	Res	Type
1	B	270	ASN
1	B	288	HIS
1	B	308	GLN
1	B	338	GLN
1	B	341	HIS
1	B	345	GLN
1	C	427	HIS
1	C	437	GLN
1	C	442	ASN
1	C	475	HIS
1	C	484	ASN
1	C	488	HIS
1	C	508	GLN
1	C	541	HIS
1	D	630	HIS
1	D	741	HIS
1	D	783	HIS
2	E	1224	ASN
2	E	1232	GLN
2	E	1238	GLN
2	E	1275	ASN
2	E	1291	GLN
2	F	1024	ASN
2	F	1032	GLN
2	F	1038	GLN
2	F	1075	ASN
2	F	1091	GLN
2	G	1612	GLN
2	G	1620	ASN
2	G	1638	GLN
2	G	1675	ASN
2	G	1691	GLN
2	H	1424	ASN
2	H	1432	GLN
2	H	1438	GLN
2	H	1475	ASN
2	H	1491	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	BFD	G	1654	2,3	8,11,12	1.31	0	3,15,17	1.86	1 (33%)
2	BFD	H	1454	2,3	8,11,12	1.25	0	3,15,17	1.95	1 (33%)
2	BFD	E	1254	2,3	8,11,12	1.40	2 (25%)	3,15,17	1.92	1 (33%)
2	BFD	F	1054	2,3	8,11,12	1.44	1 (12%)	3,15,17	2.05	1 (33%)

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	BFD	G	1654	2,3	-	1/5/11/13	-
2	BFD	H	1454	2,3	-	1/5/11/13	-
2	BFD	E	1254	2,3	-	0/5/11/13	-
2	BFD	F	1054	2,3	-	1/5/11/13	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1254	BFD	F3-BE	-2.32	1.48	1.54
2	E	1254	BFD	F1-BE	-2.20	1.48	1.54
2	F	1054	BFD	F3-BE	-2.18	1.48	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1054	BFD	OD2-CG-CB	-3.51	116.98	124.73
2	H	1454	BFD	OD2-CG-CB	-3.33	117.38	124.73
2	E	1254	BFD	OD2-CG-CB	-3.21	117.64	124.73
2	G	1654	BFD	OD2-CG-CB	-3.15	117.77	124.73

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	H	1454	BFD	O-C-CA-CB
2	F	1054	BFD	CA-CB-CG-OD2
2	G	1654	BFD	CA-CB-CG-OD1

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	1654	BFD	3	0
2	H	1454	BFD	1	0
2	E	1254	BFD	1	0
2	F	1054	BFD	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	181/192 (94%)	-0.48	2 (1%)	80	60	28, 44, 74, 91	0
1	B	182/192 (94%)	-0.47	1 (0%)	91	79	24, 46, 75, 96	3 (1%)
1	C	181/192 (94%)	-0.23	3 (1%)	70	46	42, 71, 100, 115	0
1	D	182/192 (94%)	-0.25	6 (3%)	46	23	41, 63, 98, 114	3 (1%)
2	E	118/124 (95%)	-0.13	4 (3%)	45	22	56, 78, 96, 106	0
2	F	118/124 (95%)	-0.42	1 (0%)	86	70	36, 55, 77, 87	0
2	G	118/124 (95%)	0.20	5 (4%)	36	17	75, 101, 114, 116	0
2	H	118/124 (95%)	0.02	4 (3%)	45	22	56, 87, 112, 121	1 (0%)
All	All	1198/1264 (94%)	-0.25	26 (2%)	62	38	24, 65, 107, 121	7 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	1720	PRO	6.7
1	C	413	SER	5.0
1	D	613	SER	4.8
2	H	1521	LEU	4.8
1	C	412	ILE	4.6
1	D	743	ASP	3.9
1	D	611	ASN	3.5
2	G	1721	LEU	3.1
2	G	1684	TYR	3.1
2	E	1203	ASN	3.0
1	D	612	ILE	3.0
2	H	1488	ASP	2.9
2	E	1321	LEU	2.9
2	G	1688	ASP	2.8
1	D	772	ASP	2.7
2	E	1320	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
2	G	1686	GLU	2.6
2	H	1486	GLU	2.6
1	C	414	ASP	2.5
2	F	1121	LEU	2.5
2	E	1288	ASP	2.2
1	D	615	THR	2.2
1	B	211	ASN	2.2
1	A	12	ILE	2.1
1	A	13	SER	2.1
2	H	1475	ASN	2.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BFD	H	1454	12/13	0.92	0.29	66,68,71,71	4
2	BFD	G	1654	12/13	0.93	0.17	85,87,88,88	4
2	BFD	E	1254	12/13	0.95	0.23	60,62,66,67	4
2	BFD	F	1054	12/13	0.96	0.27	39,41,42,43	4

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	G	2004	1/1	0.95	0.05	37,37,37,37	0
3	MG	H	2003	1/1	0.97	0.18	37,37,37,37	0
3	MG	F	2002	1/1	0.99	0.34	37,37,37,37	0
3	MG	E	2001	1/1	1.00	0.28	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.