



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:13 AM UTC

PDB ID : 2FTK / pdb_00002ftk
Title : beryllifluoride 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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

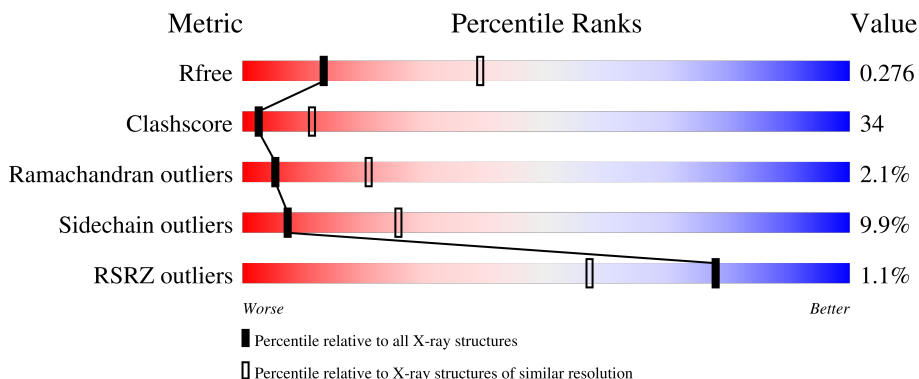
1 Overall quality at a glance i

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.




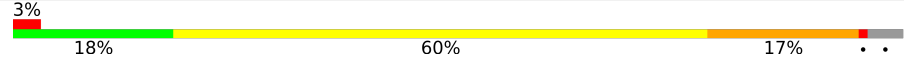

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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 $\leq 5\%$. 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	
1	B	192	
1	C	192	
1	D	192	
2	E	124	

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Mol	Chain	Length	Quality of chain
2	F	124	 <p>% 48% 42% 6% .</p>
2	G	124	 <p>3% 18% 60% 17% . .</p>
2	H	124	 <p>2% 50% 38% 8% .</p>

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
			Total	C	N	O	S			
1	A	181	1497	955	251	284	7	0	0	0
1	B	182	1505	959	253	286	7	6	0	0
1	C	181	1497	955	251	284	7	0	0	0
1	D	182	1505	959	253	286	7	6	0	0

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

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

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 (CCD ID: MG) (formula: Mg).

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

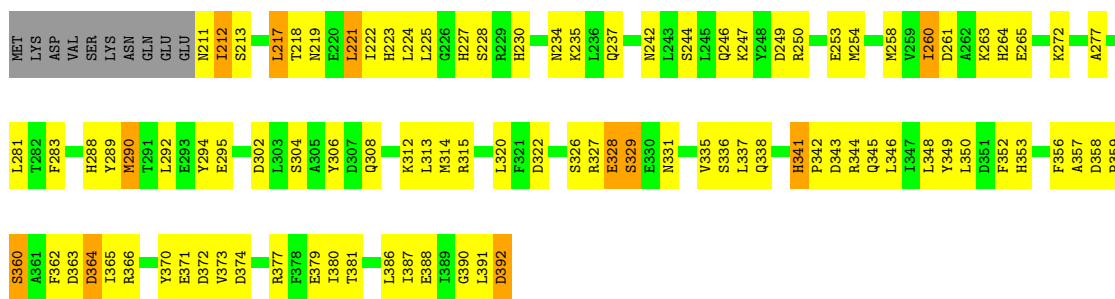
- Molecule 1: Sporulation initiation phosphotransferase B

Chain A: 

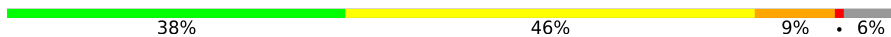


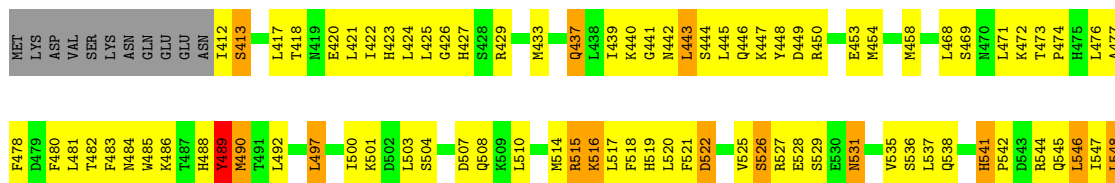
- Molecule 1: Sporulation initiation phosphotransferase B

Chain B: 



- Molecule 1: Sporulation initiation phosphotransferase B

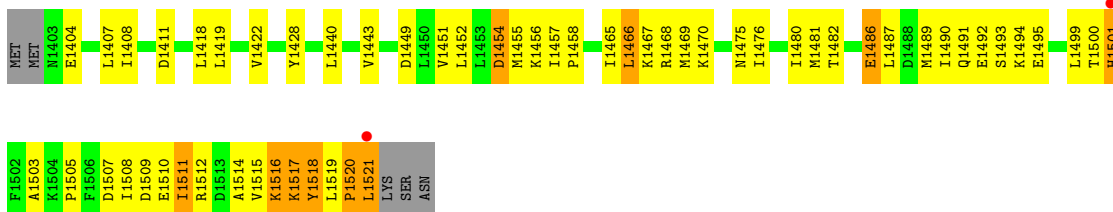
Chain C: 



SER
ASN

- Molecule 2: Sporulation initiation phosphotransferase F

Chain H: 



4 Data and refinement statistics

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) 98.2 (19.86-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 3.04Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.232 , 0.282 0.224 , 0.276	Depositor DCC
R_{free} test set	1404 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	74.1	Xtrriage
Anisotropy	0.113	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.66	0/1530	0.94	3/2064 (0.1%)
1	B	0.66	0/1538	0.97	4/2075 (0.2%)
1	C	0.55	0/1530	0.95	6/2064 (0.3%)
1	D	0.54	0/1538	0.90	1/2075 (0.0%)
2	E	0.47	0/952	0.90	2/1279 (0.2%)
2	F	0.60	0/952	0.99	3/1279 (0.2%)
2	G	0.41	0/952	1.01	5/1279 (0.4%)
2	H	0.44	0/963	0.87	1/1294 (0.1%)
All	All	0.56	0/9955	0.94	25/13409 (0.2%)

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 (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1086	GLU	N-CA-C	-8.20	100.60	110.44
2	G	1719	LEU	CA-C-N	7.40	129.09	119.84
2	G	1719	LEU	C-N-CA	7.40	129.09	119.84
1	B	341	HIS	CA-C-N	6.84	126.44	119.19
1	B	341	HIS	C-N-CA	6.84	126.44	119.19
1	A	141	HIS	CA-C-N	6.79	126.39	119.19
1	A	141	HIS	C-N-CA	6.79	126.39	119.19
1	D	757	ALA	N-CA-C	-6.67	105.70	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	357	ALA	N-CA-C	-6.59	105.81	114.31
1	C	541	HIS	CA-C-N	6.58	126.16	119.19
1	C	541	HIS	C-N-CA	6.58	126.16	119.19
1	A	157	ALA	N-CA-C	-6.46	105.98	114.31
2	G	1678	VAL	N-CA-C	6.46	117.15	108.11
1	C	557	ALA	N-CA-C	-6.23	106.27	114.31
2	H	1486	GLU	N-CA-C	-6.18	103.02	110.44
1	C	565	ILE	CB-CA-C	-6.11	104.04	112.04
2	F	1078	VAL	N-CA-C	5.73	116.13	108.11
1	C	489	TYR	N-CA-CB	-5.71	102.22	110.56
2	G	1717	LYS	N-CA-C	-5.63	105.23	111.71
2	E	1278	VAL	N-CA-C	5.53	115.83	107.75
1	C	489	TYR	CA-CB-CG	-5.32	104.33	113.90
2	E	1205	LYS	N-CA-C	5.20	117.20	109.25
2	G	1712	ARG	N-CA-C	-5.14	107.07	113.19
2	F	1046	GLU	N-CA-C	5.07	118.56	112.38
1	B	380	ILE	CB-CA-C	-5.06	104.64	110.41

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	91	0
1	B	1505	0	1463	87	0
1	C	1497	0	1457	141	0
1	D	1505	0	1463	103	0
2	E	954	0	986	45	0
2	F	954	0	986	48	0
2	G	954	0	986	137	0
2	H	964	0	992	55	0
3	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	661	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (661) 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	1.41	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:F:1051:VAL:HG11	2:F:1069:MET:HE1	1.55	0.89
2:H:1451:VAL:HG11	2:H:1469:MET:HE1	1.53	0.88
1:A:190:GLY:C	1:A:191:LEU:HD12	2.00	0.87
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
2:G:1660:MET:HE1	2:G:1664:GLU:HB3	1.61	0.83
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:433:MET:HE1	1:D:659:VAL:HG13	1.69	0.75
1:C:546:LEU:HD12	1:C:591:LEU:HD12	1.68	0.74
1:A:38:LEU:HD22	1:A:54:MET:HE1	1.70	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
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
2:G:1604:GLU:H	2:G:1604:GLU:CD	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:G:1655:MET:HE3	2:G:1689:MET:HG2	1.76	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:C:514:MET:HE1	1:C:548:LEU:CD1	2.24	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
1:B:364:ASP:OD1	1:B:364:ASP:C	2.38	0.66
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:1656:LYS:HZ3	2:G:1682:THR:HG23	1.58	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: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
1:A:74:PRO:HD2	1:A:107:ASP:OD1	1.98	0.64
1:B:327:ARG:C	2:F:1037:LEU:HD12	2.21	0.64
2:E:1286:GLU:O	2:E:1290:ILE:HG13	1.98	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:F:1055:MET:HE3	2:F:1089:MET:HB3	1.79	0.64
2:G:1657:ILE:CG2	2:G:1658:PRO:HD2	2.27	0.64
1:A:38:LEU:HD13	1:A:54:MET:HE2	1.80	0.64
1:C:471:LEU:HB2	1:C:473:THR:CG2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:H:1455:MET:HE2	2:H:1489:MET:HB3	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: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
2:G:1655:MET:CE	2:G:1689:MET:HG2	2.28	0.62
1:D:706:TYR:N	1:D:706:TYR:CD1	2.66	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: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
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: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
1:D:633:MET:HE3	1:D:633:MET:HA	1.83	0.59
2:F:1018:LEU:O	2:F:1022:VAL:HG23	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:G:1680:ILE:HG22	2:G:1681:MET:N	2.17	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:F:1086:GLU:HG3	2:F:1089:MET:HE3	1.84	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
2:G:1660:MET:CE	2:G:1664:GLU:HB3	2.30	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
1:C:549:TYR:C	1:C:550:LEU:HD12	2.29	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
1:D:749:TYR:C	1:D:750:LEU:HD12	2.29	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
1:B:386:LEU:HD13	1:B:386:LEU:C	2.30	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:H:1486:GLU:HG3	2:H:1489:MET:HE3	1.87	0.57
2:G:1717:LYS:HE3	2:G:1718:TYR:CE1	2.39	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1052:LEU:HB3	2:F:1081:MET:HE2	1.87	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: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:B:250:ARG:HE	1:B:254:MET:HE3	1.70	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:72:LYS:C	1:A:74:PRO:HD3	2.32	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:B:372:ASP:OD2	1:B:372:ASP:C	2.50	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:D:617:LEU:C	1:D:617:LEU:HD23	2.34	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: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:683:PHE:HZ	1:D:690:MET:HE3	1.74	0.53
2:G:1711:ILE:C	2:G:1713:ASP:H	2.15	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
1:C:515:ARG:HH11	1:C:515:ARG:CB	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1684:TYR:O	2:G:1685:GLY:C	2.52	0.52
1:B:349:TYR:C	1:B:350:LEU:HD12	2.34	0.52
1:D:683:PHE:CZ	1:D:690:MET:HE3	2.44	0.52
2:G:1616:ARG:NH1	2:G:1634:ALA:CB	2.72	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:C:566:ARG:HD2	1:C:578:PHE:CD1	2.45	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:514:MET:HE1	1:C:548:LEU:HD11	1.91	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
1:D:744:ARG:HE	1:D:776:MET:HE3	1.74	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
1:B:234:ASN:O	1:B:237:GLN:HB3	2.10	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
1:B:328:GLU:CD	1:B:328:GLU:O	2.54	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: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
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
1:B:250:ARG:NE	1:B:254:MET:HE3	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:314:MET:HE3	1:B:314:MET:HA	1.94	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:D:638:LEU:HG	1:D:654:MET:HE1	1.93	0.50
2:E:1251:VAL:CG1	2:E:1269:MET:HE1	2.27	0.50
2:E:1301:HIS:C	2:E:1301:HIS:CD2	2.88	0.50
1:A:38:LEU:HD13	1:A:54:MET:CE	2.40	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
1:D:694:TYR:CD1	1:D:694:TYR:C	2.89	0.50
2:E:1315:VAL:HG23	2:E:1316:LYS:N	2.26	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:B:390:GLY:C	1:B:391:LEU:HD12	2.37	0.50
1:C:449:ASP:O	1:C:453:GLU:HG3	2.12	0.50
2:H:1443:VAL:HG21	2:H:1469:MET:HE2	1.94	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:1646:GLU:O	2:G:1647:ARG:C	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:GLN:OE1	2:E:1305:PRO:HA	2.12	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
2:E:1286:GLU:HG3	2:E:1289:MET:HE3	1.94	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
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:C:546:LEU:HD13	1:C:546:LEU:C	2.38	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
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
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
2:G:1715:VAL:HG23	2:G:1716:LYS:H	1.78	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:G:1620:ASN:C	2:G:1622:VAL:H	2.22	0.47
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
1:A:93:GLU:HB2	1:A:132:HIS:NE2	2.28	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:1637:LEU:C	2:G:1639:ALA:N	2.69	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:650:ARG:HH21	1:D:654:MET:HE3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:738:GLN:O	1:D:746:LEU:HD23	2.15	0.47
2:H:1507:ASP:C	2:H:1509:ASP:N	2.72	0.47
2:G:1637:LEU:C	2:G:1639:ALA:H	2.23	0.47
2:H:1428:TYR:CE1	2:H:1519:LEU:HD23	2.49	0.47
2:F:1011:ASP:HB3	2:F:1058:PRO:HD2	1.97	0.47
2:F:1107:ASP:C	2:F:1109:ASP:N	2.71	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:B:244:SER:C	1:B:246:GLN:H	2.24	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
1:D:633:MET:HE2	1:D:636:LEU:HD12	1.96	0.46
2:G:1604:GLU:HB2	2:G:1649:ASP:OD1	2.15	0.46
2:G:1620:ASN:CG	2:G:1632:GLN:HE21	2.19	0.46
2:G:1640:LEU:HD23	2:G:1640:LEU:C	2.41	0.46
2:G:1667:LYS:O	2:G:1671:VAL:HG23	2.15	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:H:1452:LEU:HB3	2:H:1481:MET:HE2	1.97	0.46
2:H:1491:GLN:HA	2:H:1491:GLN:NE2	2.31	0.46
1:D:762:PHE:O	1:D:766:ARG:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1646:GLU:O	2:G:1646:GLU:CD	2.58	0.45
1:C:443:LEU:HD22	1:C:443:LEU:O	2.15	0.45
1:D:716:LYS:HD3	1:D:716:LYS:C	2.41	0.45
2:E:1275:ASN:HD22	2:E:1275:ASN:N	2.13	0.45
2:G:1668:ARG:O	2:G:1669:MET:C	2.59	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
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: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:O	1:D:780:ILE:HG12	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
1:A:44:SER:C	1:A:46:GLN:H	2.25	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:526:SER:C	1:C:527:ARG:HD2	2.43	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:302:ASP:OD2	1:B:302:ASP:C	2.60	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
1:A:147:ILE:HG22	1:A:148:LEU:N	2.33	0.44
1:D:762:PHE:O	1:D:763:ASP:C	2.60	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
2:G:1652:LEU:C	2:G:1681:MET:HE2	2.43	0.44
1:C:439:ILE:HG13	1:C:458:MET:HE1	1.99	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
2:G:1711:ILE:C	2:G:1713:ASP:N	2.74	0.44
1:C:417:LEU:C	1:C:417:LEU:HD23	2.42	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:437:GLN:NE2	1:C:437:GLN:C	2.76	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:C:478:PHE:CE2	1:D:621:LEU:CD2	3.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:771:GLU:CG	1:D:772:ASP:H	2.29	0.43
2:F:1043:VAL:HG21	2:F:1069:MET:HE2	2.00	0.43
1:C:515:ARG:CB	1:C:515:ARG:NH1	2.81	0.43
1:C:433:MET:HE3	2:G:1705:PRO:HD2	2.01	0.43
2:F:1080:ILE:HD13	2:F:1093:SER:OG	2.18	0.43
2:F:1107:ASP:C	2:F:1109:ASP:H	2.27	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
2:G:1619:LEU:O	2:G:1620:ASN:C	2.61	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:HD2	1:C:527:ARG:N	2.34	0.42
1:B:272:LYS:HE2	1:B:304:SER:HB3	2.01	0.42
1:B:362:PHE:O	1:B:363:ASP:C	2.61	0.42
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:E:1276:ILE:HG23	2:E:1276:ILE:O	2.18	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
1:A:167:GLN:C	1:A:168:ASN:HD22	2.26	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
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:G:1661:ASP:C	2:G:1663:ILE:H	2.27	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:E:1307:ASP:C	2:E:1309:ASP:N	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:C:514:MET:HE1	1:C:548:LEU:HD13	1.99	0.42
1:D:644:SER:C	1:D:646:GLN:H	2.26	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: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:1654:BFD:CG	2:G:1655:MET:H	2.33	0.41
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:C:473:THR:HA	1:C:507:ASP:CG	2.44	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:H:1452:LEU:N	2:H:1452:LEU:HD12	2.35	0.41
2:H:1507:ASP:C	2:H:1509:ASP:H	2.28	0.41
1:B:306:TYR:OH	1:B:345:GLN:HG2	2.20	0.41
1:D:627:HIS:O	1:D:628:SER:C	2.63	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
1:D:779:GLU:C	1:D:780:ILE:HG22	2.45	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
1:A:170:TYR:O	1:A:171:GLU:C	2.63	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:C:562:PHE:O	1:C:563:ASP:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:HIS:O	1:A:28:SER:C	2.61	0.41
1:A:162:PHE:CD1	1:A:178:PHE:HZ	2.39	0.41
1:B:227:HIS:O	1:B:228:SER:C	2.63	0.41
1:B:230:HIS:CD2	2:F:1083:ALA:HB3	2.56	0.41
1:B:314:MET:HE3	1:B:314:MET:CA	2.50	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:444:SER:C	1:C:446:GLN:H	2.28	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: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:B:224:LEU:O	1:B:225:LEU:C	2.64	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:737:LEU:HG	1:D:748:LEU:CD1	2.51	0.41
2:G:1699:LEU:O	2:G:1700:THR:HB	2.19	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:H:1466:LEU:HD22	2:H:1466:LEU:O	2.20	0.40
2:H:1517:LYS:C	2:H:1519:LEU:H	2.29	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
1:D:770:TYR:O	1:D:771:GLU:C	2.64	0.40
2:F:1046:GLU:O	2:F:1047:ARG:C	2.63	0.40
2:G:1623:PHE:HZ	2:G:1711:ILE:HG23	1.86	0.40
1:A:162:PHE:O	1:A:163:ASP:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:MET:HE2	1:B:290:MET:HB3	1.92	0.40
1:D:770:TYR:O	1:D:773:VAL:HG22	2.21	0.40
2:H:1512:ARG:C	2:H:1515:VAL:HG22	2.46	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:F:1112:ARG:C	2:F:1115:VAL:HG22	2.46	0.40
2:G:1623:PHE:CE1	2:G:1715:VAL:HG21	2.56	0.40
2:H:1475:ASN:N	2:H:1475:ASN:ND2	2.67	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
1:C:570:TYR:O	1:C:571:GLU:C	2.64	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%)	11	34
1	B	180/192 (94%)	166 (92%)	13 (7%)	1 (1%)	21	48
1	C	179/192 (93%)	165 (92%)	12 (7%)	2 (1%)	11	34
1	D	180/192 (94%)	168 (93%)	11 (6%)	1 (1%)	21	48
2	E	116/124 (94%)	100 (86%)	15 (13%)	1 (1%)	14	39
2	F	116/124 (94%)	99 (85%)	14 (12%)	3 (3%)	4	17
2	G	116/124 (94%)	84 (72%)	20 (17%)	12 (10%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	117/124 (94%)	100 (86%)	14 (12%)	3 (3%)	4	17
All	All	1183/1264 (94%)	1047 (88%)	111 (9%)	25 (2%)	5	21

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%)	149 (90%)	17 (10%)	7	24
1	B	167/177 (94%)	152 (91%)	15 (9%)	9	29
1	C	166/177 (94%)	143 (86%)	23 (14%)	3	13
1	D	167/177 (94%)	147 (88%)	20 (12%)	5	17
2	E	104/109 (95%)	96 (92%)	8 (8%)	12	35
2	F	104/109 (95%)	97 (93%)	7 (7%)	15	39
2	G	104/109 (95%)	94 (90%)	10 (10%)	8	26
2	H	105/109 (96%)	97 (92%)	8 (8%)	12	35
All	All	1083/1144 (95%)	975 (90%)	108 (10%)	7	25

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ILE
1	A	17	LEU
1	A	43	LEU
1	A	45	LEU
1	A	49	ASP
1	A	50	ARG
1	A	66	SER
1	A	81	LEU
1	A	93	GLU
1	A	116	LYS
1	A	145	GLN
1	A	148	LEU
1	A	151	ASP
1	A	165	ILE
1	A	166	ARG
1	A	180	ILE
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	247	LYS
1	B	260	ILE
1	B	290	MET
1	B	328	GLU
1	B	329	SER

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Mol	Chain	Res	Type
1	B	336	SER
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	440	LYS
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	516	LYS
1	C	522	ASP
1	C	526	SER
1	C	531	ASN
1	C	546	LEU
1	C	548	LEU
1	C	549	TYR
1	C	551	ASP
1	C	564	ASP
1	C	565	ILE
1	C	566	ARG
1	C	580	ILE
1	C	582	SER
1	C	586	LEU
1	D	617	LEU
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	700	ILE
1	D	706	TYR
1	D	709	LYS
1	D	716	LYS
1	D	723	GLN
1	D	726	SER

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Mol	Chain	Res	Type
1	D	736	SER
1	D	746	LEU
1	D	765	ILE
1	D	768	ASN
1	D	779	GLU
1	D	780	ILE
2	E	1204	GLU
2	E	1265	ILE
2	E	1266	LEU
2	E	1286	GLU
2	E	1292	GLU
2	E	1311	ILE
2	E	1316	LYS
2	E	1321	LEU
2	F	1004	GLU
2	F	1065	ILE
2	F	1066	LEU
2	F	1092	GLU
2	F	1111	ILE
2	F	1116	LYS
2	F	1121	LEU
2	G	1605	LYS
2	G	1612	GLN
2	G	1650	LEU
2	G	1652	LEU
2	G	1663	ILE
2	G	1669	MET
2	G	1682	THR
2	G	1690	ILE
2	G	1699	LEU
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 (56) 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	131	ASN
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	264	HIS
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	B	367	GLN
1	C	427	HIS
1	C	430	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	531	ASN
1	C	541	HIS
1	D	630	HIS
1	D	675	HIS
1	D	732	HIS
1	D	741	HIS
1	D	753	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

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Mol	Chain	Res	Type
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 [i](#)

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	H	1454	3,2	8,11,12	1.29	0	2,15,17	2.22	1 (50%)
2	BFD	F	1054	3,2	8,11,12	1.49	2 (25%)	2,15,17	2.36	1 (50%)
2	BFD	G	1654	3,2	8,11,12	1.35	0	2,15,17	2.11	1 (50%)
2	BFD	E	1254	3,2	8,11,12	1.46	2 (25%)	2,15,17	2.13	1 (50%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	BFD	H	1454	3,2	-	1/5/11/13	-
2	BFD	F	1054	3,2	-	1/5/11/13	-
2	BFD	G	1654	3,2	-	0/5/11/13	-
2	BFD	E	1254	3,2	-	0/5/11/13	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1254	BFD	F3-BE	-2.44	1.48	1.54
2	E	1254	BFD	F1-BE	-2.31	1.48	1.54
2	F	1054	BFD	F3-BE	-2.29	1.48	1.54
2	F	1054	BFD	F1-BE	-2.09	1.49	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1054	BFD	OD2-CG-CB	-3.30	116.98	124.65
2	H	1454	BFD	OD2-CG-CB	-3.13	117.38	124.65
2	E	1254	BFD	OD2-CG-CB	-3.02	117.64	124.65
2	G	1654	BFD	OD2-CG-CB	-2.96	117.77	124.65

There are no chirality outliers.

All (2) 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

There are no ring outliers.

4 monomers are involved in 6 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

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

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, 95th 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%)	-0.56	1 (0%) 85 69	28, 44, 74, 91	0
1	B	182/192 (94%)	-0.52	0 100 100	24, 46, 75, 96	3 (1%)
1	C	181/192 (94%)	-0.29	0 100 100	42, 71, 100, 115	0
1	D	182/192 (94%)	-0.26	4 (2%) 62 39	41, 63, 98, 114	3 (1%)
2	E	118/124 (95%)	-0.24	1 (0%) 82 63	56, 78, 96, 106	0
2	F	118/124 (95%)	-0.45	1 (0%) 82 63	36, 55, 77, 87	0
2	G	118/124 (95%)	0.08	4 (3%) 48 27	68, 91, 103, 104	0
2	H	118/124 (95%)	0.05	2 (1%) 69 46	34, 87, 112, 121	1 (0%)
All	All	1198/1264 (94%)	-0.30	13 (1%) 78 57	24, 64, 101, 121	7 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	1501[A]	HIS	10.1
2	G	1721	LEU	3.1
2	G	1720	PRO	3.1
1	D	743	ASP	2.9
2	E	1321	LEU	2.4
2	G	1684	TYR	2.3
2	G	1719	LEU	2.3
1	D	613	SER	2.2
1	A	12	ILE	2.2
1	D	612	ILE	2.2
2	H	1521	LEU	2.2
2	F	1120	PRO	2.1
1	D	617	LEU	2.0

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, 95th 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(\AA^2)	Q<0.9
2	BFD	G	1654	12/13	0.74	0.10	85,87,88,88	4
2	BFD	H	1454	12/13	0.79	0.11	66,68,71,71	4
2	BFD	E	1254	12/13	0.93	0.07	60,62,66,67	4
2	BFD	F	1054	12/13	0.93	0.09	39,41,42,43	4

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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(\AA^2)	Q<0.9
3	MG	H	2003	1/1	0.94	0.11	37,37,37,37	0
3	MG	F	2002	1/1	0.96	0.21	37,37,37,37	0
3	MG	E	2001	1/1	0.97	0.14	37,37,37,37	0
3	MG	G	2004	1/1	0.98	0.04	37,37,37,37	0

6.5 Other polymers [i](#)

There are no such residues in this entry.