



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2026 – 02:39 PM UTC

PDB ID : 3G6J / pdb_00003g6j
Title : C3b in complex with a C3b specific Fab
Authors : Wiesmann, C.
Deposited on : 2009-02-06
Resolution : 3.10 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
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

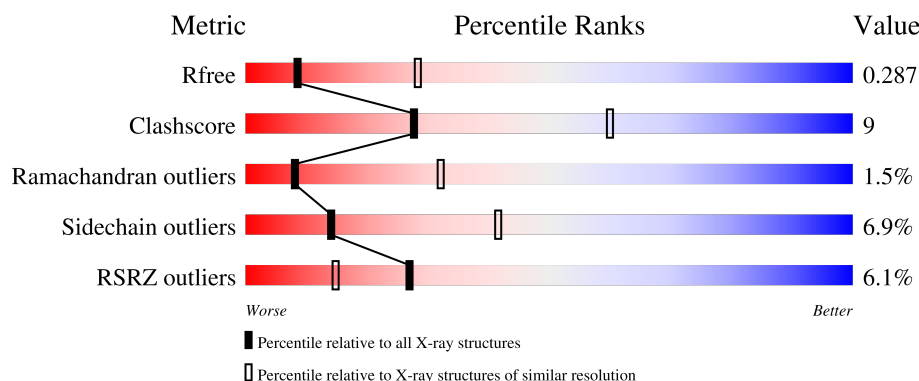
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	644	
1	C	644	
2	B	915	
2	D	915	
3	E	214	

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Mol	Chain	Length	Quality of chain
3	G	214	 74%21%5%
4	F	226	 76%19%••
4	H	226	 81%14%••

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 31008 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 Complement C3 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	642	Total	C	N	O	S	0	0	0
			5007	3187	848	957	15			
1	C	642	Total	C	N	O	S	0	0	0
			5007	3187	848	957	15			

- Molecule 2 is a protein called Complement C3 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	903	Total	C	N	O	S	0	0	0
			7213	4572	1213	1390	38			
2	D	903	Total	C	N	O	S	0	0	0
			7213	4572	1213	1390	38			

- Molecule 3 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	214	Total	C	N	O	S	0	0	0
			1640	1027	271	336	6			
3	G	214	Total	C	N	O	S	0	0	0
			1640	1027	271	336	6			

- Molecule 4 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	221	Total	C	N	O	S	0	0	0
			1643	1041	271	324	7			
4	H	221	Total	C	N	O	S	0	0	0
			1643	1041	271	324	7			

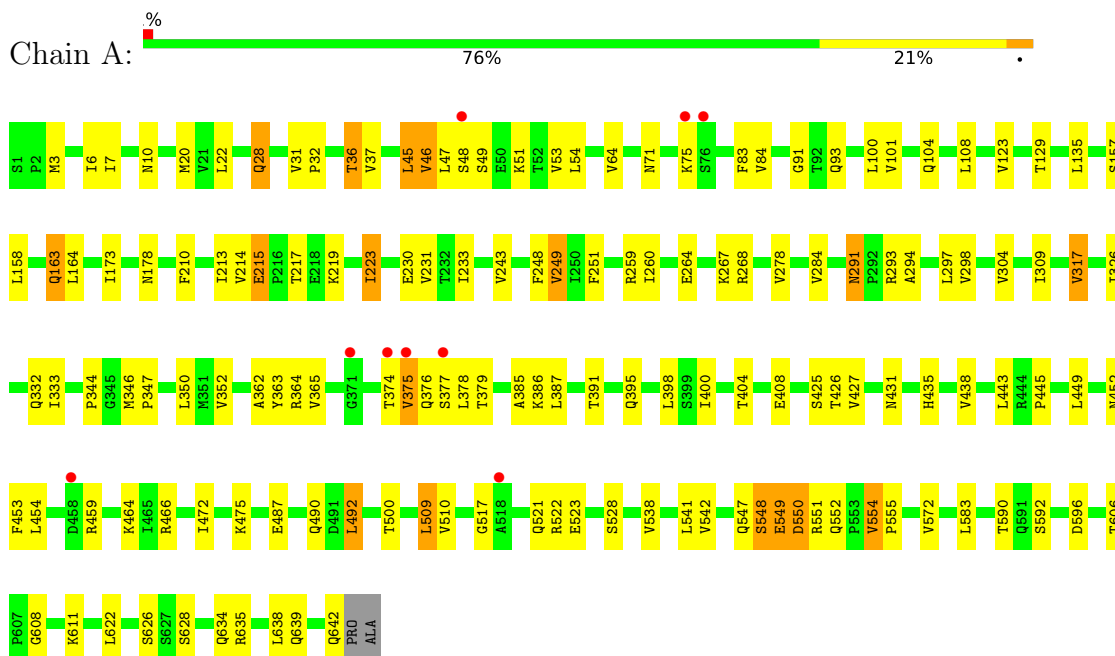
- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

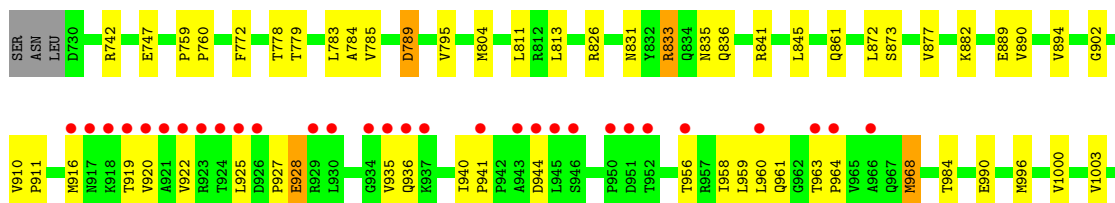
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Ca 1	0	0
5	C	1	Total 1	Ca 1	0	0

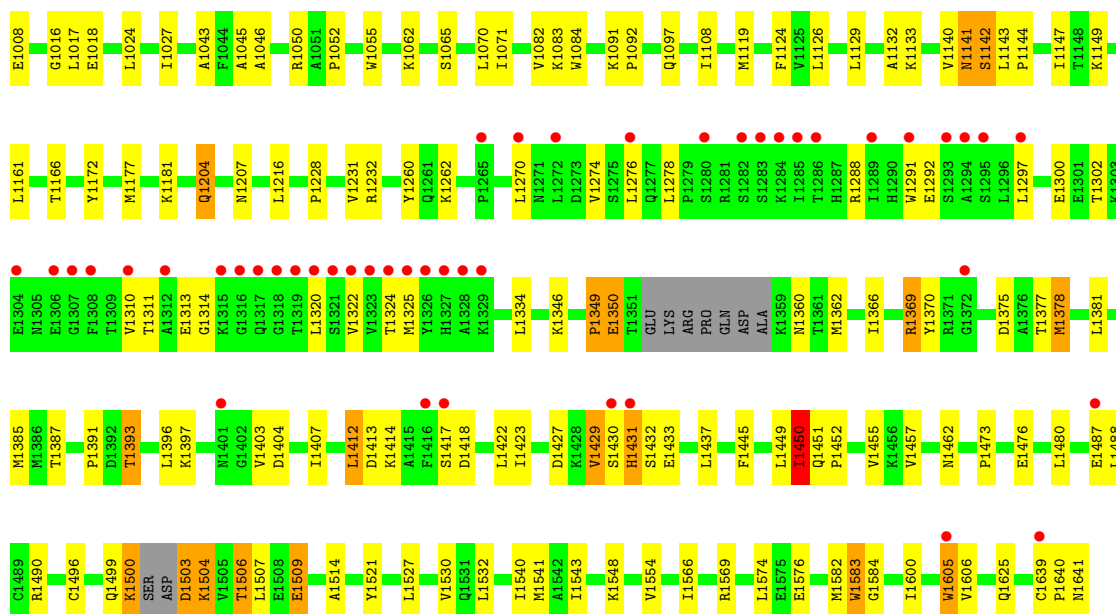
3 Residue-property plots

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: Complement C3 beta chain

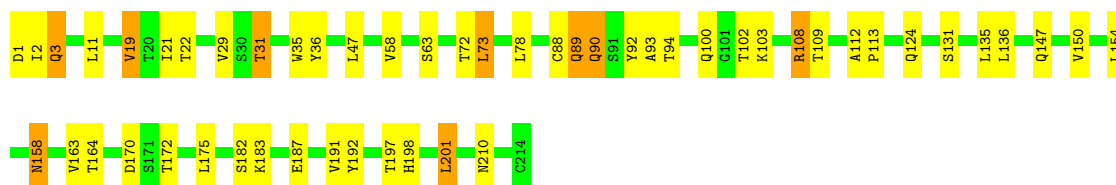






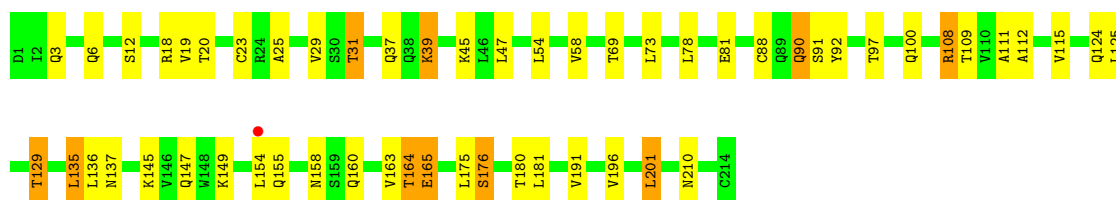
• Molecule 3: Fab light chain

Chain E: 76% 20% .



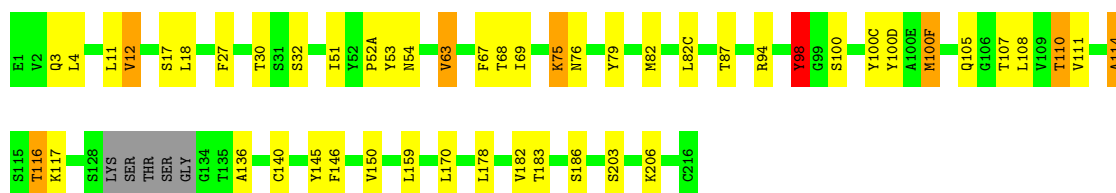
• Molecule 3: Fab light chain

Chain G: 74% 21% 5%



• Molecule 4: Fab heavy chain

Chain F: 76% 19% . .



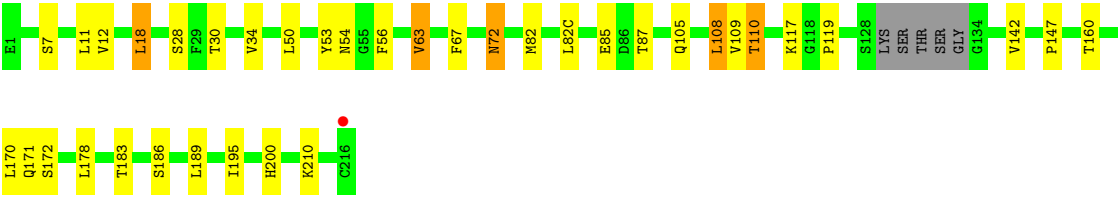
• Molecule 4: Fab heavy chain

Chain H:

81%

14%

• •



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	216.44Å 180.42Å 154.58Å 90.00° 115.73° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 20.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-3.10) 99.6 (20.00-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.01	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.214 , 0.282 0.225 , 0.287	Depositor DCC
R_{free} test set	4843 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	48.4	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	31008	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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: CA

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	0.48	0/5108	0.69	0/6940
1	C	0.48	0/5108	0.70	0/6940
2	B	0.51	1/7356 (0.0%)	0.74	8/9958 (0.1%)
2	D	0.49	0/7356	0.75	0/9958
3	E	0.49	0/1675	0.71	0/2276
3	G	0.53	0/1675	0.72	0/2276
4	F	0.50	0/1684	0.71	1/2294 (0.0%)
4	H	0.51	0/1684	0.75	0/2294
All	All	0.49	1/31646 (0.0%)	0.72	9/42936 (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
2	B	0	3
2	D	0	1
4	H	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	912	GLU	CA-C	6.31	1.55	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1268	GLN	N-CA-C	10.95	128.01	111.04
2	B	965	VAL	N-CA-C	-6.74	106.16	112.83
4	F	98	TYR	N-CA-C	6.13	123.86	110.80
2	B	1269	GLU	N-CA-C	5.58	117.11	109.18
2	B	1516	GLU	CA-C-N	5.46	126.66	119.84
2	B	1516	GLU	C-N-CA	5.46	126.66	119.84
2	B	1430	SER	CB-CA-C	-5.43	107.61	114.40
2	B	1228	PRO	N-CA-C	5.41	117.29	110.70
2	B	967	GLN	N-CA-C	-5.15	104.88	110.91

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1267	HIS	Peptide
2	B	1268	GLN	Peptide
2	B	964	PRO	Peptide
1	C	40	PHE	Peptide
2	D	1639	CYS	Peptide
4	H	53	TYR	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	5007	0	5068	104	0
1	C	5007	0	5068	104	0
2	B	7213	0	7142	129	0
2	D	7213	0	7140	128	0
3	E	1640	0	1591	31	0
3	G	1640	0	1591	36	0
4	F	1643	0	1593	31	0
4	H	1643	0	1593	30	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
All	All	31008	0	30786	553	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 9.

All (553) 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)
4:F:82:MET:HE2	4:F:82(C):LEU:HD21	1.11	1.05
4:H:82:MET:HE2	4:H:82(C):LEU:HD21	1.39	1.03
2:B:1381:LEU:CD2	2:B:1457:VAL:HG12	1.90	1.01
3:E:90:GLN:NE2	3:E:92:TYR:O	1.92	1.00
4:F:82:MET:HE2	4:F:82(C):LEU:CD2	1.98	0.94
2:B:1543:ILE:HD12	2:B:1554:VAL:HG21	1.52	0.91
1:A:249:VAL:HG21	1:A:278:VAL:HG11	1.55	0.88
1:C:151:ILE:HG21	2:D:1297:LEU:HD13	1.55	0.88
1:A:20:MET:HE2	1:A:22:LEU:HD21	1.56	0.88
1:A:268:ARG:HB2	2:B:1378:MET:HE3	1.56	0.86
4:H:82:MET:CE	4:H:82(C):LEU:HD21	2.06	0.85
1:A:28:GLN:HA	1:A:28:GLN:HE21	1.43	0.84
2:D:1381:LEU:HD23	2:D:1457:VAL:HG12	1.60	0.84
1:C:290:GLN:C	1:C:292:PRO:CD	2.53	0.81
1:C:443:LEU:HD21	1:C:499:ILE:HG13	1.62	0.80
1:A:346:MET:HE3	1:A:454:LEU:HD23	1.63	0.80
2:B:1572:LEU:HD22	2:B:1574:LEU:HD21	1.65	0.79
3:G:112:ALA:HB1	3:G:201:LEU:HD13	1.64	0.79
3:G:147:GLN:CD	3:G:154:LEU:HD11	2.07	0.78
4:F:63:VAL:HG13	4:F:67:PHE:HB2	1.66	0.77
1:C:438:VAL:HG13	1:C:449:LEU:HD11	1.65	0.77
2:B:1381:LEU:HD23	2:B:1457:VAL:HG12	1.68	0.76
1:C:293:ARG:HH11	1:C:293:ARG:CG	1.99	0.75
2:B:1543:ILE:CD1	2:B:1554:VAL:HG21	2.15	0.75
1:C:293:ARG:HH11	1:C:293:ARG:HG2	1.51	0.75
1:C:290:GLN:C	1:C:292:PRO:HD2	2.12	0.75
1:A:438:VAL:HG11	1:A:449:LEU:HD21	1.67	0.75
1:C:290:GLN:O	1:C:292:PRO:HD2	1.89	0.72
1:C:291:ASN:N	1:C:292:PRO:CD	2.53	0.72
1:A:3:MET:HE2	1:A:626:SER:CB	2.19	0.72
2:D:785:VAL:HG22	2:D:795:VAL:HG22	1.72	0.71
1:C:290:GLN:C	1:C:292:PRO:HD3	2.15	0.71
3:G:29:VAL:HG13	3:G:92:TYR:HB2	1.71	0.71
3:G:180:THR:O	3:G:181:LEU:HD13	1.91	0.71
2:B:1543:ILE:HD12	2:B:1554:VAL:CG2	2.20	0.71
1:C:293:ARG:HG2	1:C:293:ARG:NH1	2.04	0.70
1:C:3:MET:HE3	1:C:628:SER:OG	1.91	0.70
2:D:1527:LEU:HD21	2:D:1530:VAL:HG22	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:LEU:CD2	1:A:129:THR:HG22	2.22	0.69
1:C:6:ILE:HB	1:C:20:MET:HE3	1.75	0.68
2:D:1404:ASP:HA	2:D:1427:ASP:CG	2.20	0.67
2:D:811:LEU:HG	2:D:813:LEU:HD13	1.77	0.67
2:B:925:LEU:HD22	2:B:1312:ALA:HB2	1.77	0.67
4:F:67:PHE:CZ	4:F:82:MET:HE3	2.30	0.66
1:A:6:ILE:HD12	1:A:6:ILE:O	1.94	0.66
2:D:1504:LYS:O	2:D:1504:LYS:HG2	1.93	0.66
1:A:347:PRO:HG2	1:C:492:LEU:HD22	1.78	0.66
2:B:1369:ARG:HA	2:B:1429:VAL:CG2	2.26	0.66
3:G:137:ASN:HD21	4:H:183:THR:HG21	1.61	0.66
2:D:1527:LEU:HD13	2:D:1541:MET:HE2	1.78	0.66
2:B:1068:VAL:HG23	2:B:1069:ASN:HD22	1.60	0.65
1:C:249:VAL:CG2	1:C:278:VAL:HG21	2.26	0.65
1:C:6:ILE:CB	1:C:20:MET:HE3	2.26	0.65
1:C:465:ILE:HD11	1:C:515:LEU:HD13	1.77	0.65
3:E:2:ILE:HD12	3:E:93:ALA:HB2	1.78	0.65
1:A:231:VAL:HG21	1:A:304:VAL:HG21	1.79	0.65
2:B:1411:GLU:HG2	2:B:1422:LEU:HD12	1.79	0.65
2:D:1543:ILE:HD12	2:D:1554:VAL:HG21	1.79	0.64
2:D:1521:TYR:CZ	2:D:1584:GLY:HA3	2.32	0.64
2:D:1422:LEU:HD12	2:D:1423:ILE:N	2.13	0.64
1:C:40:PHE:O	1:C:40:PHE:CD2	2.51	0.64
2:D:968:MET:HE2	2:D:968:MET:HA	1.79	0.63
2:B:914:ILE:HD13	2:B:915:ARG:H	1.64	0.63
3:E:92:TYR:O	3:E:93:ALA:HB3	1.97	0.63
2:B:1528:VAL:HG21	2:B:1559:GLN:HE21	1.64	0.63
1:C:348:PHE:CE2	1:C:350:LEU:HD12	2.34	0.63
1:A:3:MET:HE2	1:A:626:SER:OG	1.98	0.63
1:A:293:ARG:O	1:A:294:ALA:C	2.41	0.63
1:C:291:ASN:O	1:C:293:ARG:N	2.32	0.63
2:B:1284:LYS:O	2:B:1285:ILE:HD13	1.98	0.63
2:D:1147:ILE:CG2	2:D:1177:MET:HE2	2.29	0.63
3:E:29:VAL:CG1	3:E:29:VAL:O	2.47	0.62
3:E:124:GLN:HE22	3:E:131:SER:CB	2.12	0.62
1:C:291:ASN:N	1:C:292:PRO:HD3	2.14	0.62
1:A:249:VAL:CG2	1:A:278:VAL:HG21	2.30	0.62
1:C:253:ILE:HD11	1:C:262:LEU:HD11	1.80	0.62
3:G:160:GLN:HE22	4:H:171:GLN:HA	1.64	0.62
4:H:63:VAL:HG21	4:H:67:PHE:CD2	2.35	0.62
2:B:1381:LEU:HD21	2:B:1457:VAL:HG12	1.79	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:910:VAL:HG13	2:D:911:PRO:HD2	1.81	0.61
1:C:249:VAL:HG21	1:C:278:VAL:HG21	1.81	0.61
1:A:248:PHE:HE2	1:A:309:ILE:HD12	1.64	0.61
1:C:100:LEU:HD21	1:C:638:LEU:HD23	1.82	0.61
1:C:573:LEU:HD23	2:D:784:ALA:HB2	1.83	0.61
2:B:835:ASN:HB3	4:F:54:ASN:HD21	1.66	0.60
2:B:967:GLN:O	2:B:969:THR:N	2.35	0.60
2:D:1437:LEU:C	2:D:1437:LEU:HD12	2.26	0.60
2:D:1387:THR:HG23	2:D:1451:GLN:H	1.65	0.60
3:E:29:VAL:O	3:E:29:VAL:HG12	2.01	0.60
1:A:223:ILE:HG23	1:A:326:ILE:CG2	2.32	0.60
2:B:1507:LEU:HD11	2:B:1629:ALA:HB1	1.84	0.59
2:B:1447:VAL:HG13	2:B:1450:ILE:HG22	1.84	0.59
3:E:36:TYR:OH	3:E:89:GLN:NE2	2.35	0.59
2:D:1362:MET:HE1	2:D:1473:PRO:HB3	1.84	0.59
1:A:346:MET:CE	1:A:454:LEU:HD23	2.30	0.59
1:A:251:PHE:CE1	1:A:304:VAL:HG22	2.38	0.59
2:B:1056:LEU:O	2:B:1060:VAL:HG23	2.03	0.59
1:C:214:VAL:HG12	1:C:233:ILE:HD12	1.84	0.59
4:F:145:TYR:CE2	4:F:150:VAL:HG23	2.37	0.59
1:A:572:VAL:HG12	2:B:753:VAL:HG22	1.83	0.59
4:F:12:VAL:HG23	4:F:111:VAL:HG22	1.84	0.59
1:C:293:ARG:O	1:C:295:GLU:N	2.36	0.59
3:G:164:THR:HG23	3:G:165:GLU:O	2.02	0.59
1:A:365:VAL:H	1:A:379:THR:HG22	1.67	0.59
2:B:1370:TYR:N	2:B:1430:SER:O	2.35	0.59
1:A:391:THR:HG22	1:A:398:LEU:HD11	1.83	0.59
2:D:1521:TYR:CE2	2:D:1584:GLY:HA3	2.38	0.58
1:C:210:PHE:CE1	1:C:317:VAL:CG1	2.87	0.58
3:G:54:LEU:HD11	3:G:58:VAL:CG1	2.33	0.58
1:A:6:ILE:HD12	1:A:6:ILE:C	2.29	0.58
2:B:1375:ASP:CG	2:B:1430:SER:HB2	2.28	0.58
2:D:919:THR:HG21	2:D:922:VAL:HG13	1.85	0.58
2:D:1274:VAL:HG13	2:D:1311:THR:O	2.03	0.58
2:D:916:MET:HE2	2:D:916:MET:HA	1.85	0.58
1:C:223:ILE:HD11	1:C:328:THR:HG22	1.85	0.58
3:E:112:ALA:HB1	3:E:201:LEU:CD1	2.34	0.58
3:G:29:VAL:O	3:G:29:VAL:HG12	2.03	0.58
1:C:293:ARG:O	1:C:294:ALA:C	2.46	0.57
2:D:1065:SER:OG	2:D:1132:ALA:HB2	2.03	0.57
2:B:1518:GLY:HA3	2:B:1585:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:31:THR:O	3:G:31:THR:CG2	2.52	0.57
1:C:36:THR:HG23	1:C:87:GLN:HB3	1.87	0.57
3:E:163:VAL:HG22	3:E:175:LEU:HD12	1.86	0.57
4:F:63:VAL:HG22	4:F:67:PHE:CG	2.40	0.57
4:H:72:ASN:HD22	4:H:72:ASN:C	2.12	0.57
2:B:1155:GLU:O	2:B:1184:LEU:HD21	2.05	0.57
2:D:1082:VAL:HG13	2:D:1129:LEU:CD2	2.34	0.57
1:A:350:LEU:HD12	1:A:400:ILE:HD13	1.86	0.57
2:B:1334:LEU:HG	2:B:1335:THR:HG23	1.86	0.57
2:D:1381:LEU:CD2	2:D:1457:VAL:HG12	2.33	0.56
2:D:1055:TRP:CE2	2:D:1108:ILE:HG22	2.40	0.56
2:B:1215:LEU:HD21	2:B:1231:VAL:HG22	1.87	0.56
1:C:249:VAL:HG21	1:C:278:VAL:HG11	1.85	0.56
2:D:1393:THR:HG22	2:D:1397:LYS:HD2	1.87	0.56
1:A:3:MET:HE2	1:A:626:SER:HB2	1.87	0.56
2:B:1147:ILE:HG23	2:B:1177:MET:HE2	1.87	0.56
1:A:554:VAL:HG13	1:A:555:PRO:HD2	1.88	0.56
2:B:924:THR:HG23	2:B:1317:GLN:HG3	1.88	0.56
1:C:214:VAL:HG12	1:C:233:ILE:CD1	2.36	0.56
2:D:1543:ILE:CD1	2:D:1554:VAL:HG21	2.35	0.56
1:C:223:ILE:HD13	1:C:298:VAL:CG2	2.35	0.56
1:C:484:GLN:OE1	1:C:495:LEU:HD13	2.06	0.55
2:B:1122:THR:HB	2:B:1154:LEU:HD21	1.88	0.55
1:C:291:ASN:O	1:C:292:PRO:C	2.49	0.55
1:C:573:LEU:CD2	2:D:784:ALA:HB2	2.35	0.55
4:H:63:VAL:HG22	4:H:67:PHE:CG	2.41	0.55
1:A:100:LEU:HD21	1:A:638:LEU:HG	1.89	0.55
2:B:968:MET:HE2	2:B:968:MET:HA	1.87	0.55
1:C:82:LYS:HZ2	1:C:103:LEU:HD11	1.72	0.55
2:D:877:VAL:HG23	2:D:1480:LEU:HD11	1.89	0.55
1:A:606:THR:HG22	1:A:608:GLY:H	1.72	0.54
3:E:19:VAL:HG21	3:E:78:LEU:HD13	1.89	0.54
1:A:362:ALA:HB1	1:A:365:VAL:HG21	1.90	0.54
1:A:510:VAL:HG22	1:A:528:SER:HB3	1.88	0.54
1:C:214:VAL:HG23	1:C:214:VAL:O	2.08	0.54
3:E:47:LEU:HA	3:E:58:VAL:HG21	1.88	0.54
1:A:210:PHE:CZ	1:A:317:VAL:HG13	2.43	0.54
1:A:346:MET:HE1	1:A:435:HIS:CD2	2.43	0.54
2:B:1027:ILE:HG22	2:B:1071:ILE:HD13	1.89	0.54
2:D:835:ASN:CB	4:H:54:ASN:ND2	2.71	0.54
1:A:249:VAL:HG21	1:A:278:VAL:HG21	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1270:LEU:HD23	2:B:1316:GLY:HA2	1.90	0.54
4:F:82:MET:CE	4:F:82(C):LEU:HD21	2.07	0.54
3:G:6:GLN:O	3:G:100:GLN:NE2	2.41	0.54
3:G:108:ARG:HD3	3:G:109:THR:O	2.08	0.54
1:A:84:VAL:HG13	1:A:101:VAL:HG21	1.89	0.53
1:C:472:ILE:HG12	1:C:509:LEU:HD22	1.89	0.53
2:D:1082:VAL:HG13	2:D:1129:LEU:HD22	1.90	0.53
4:F:17:SER:HB2	4:H:72:ASN:HD21	1.73	0.53
4:F:87:THR:HG23	4:F:110:THR:HA	1.91	0.53
4:H:54:ASN:HD22	4:H:56:PHE:HB2	1.73	0.53
2:D:1370:TYR:O	2:D:1431:HIS:HB2	2.08	0.53
4:H:87:THR:HG23	4:H:110:THR:HA	1.90	0.53
2:D:964:PRO:HB3	2:D:1270:LEU:HD11	1.89	0.53
2:D:1369:ARG:HG2	2:D:1430:SER:O	2.09	0.53
2:B:773:LEU:HD13	2:B:803:VAL:HG22	1.91	0.53
2:D:1375:ASP:CG	2:D:1430:SER:HB2	2.34	0.53
2:D:845:LEU:HD22	2:D:889:GLU:HG2	1.91	0.53
2:D:1385:MET:HE2	2:D:1385:MET:HA	1.90	0.53
1:A:45:LEU:HD22	1:A:45:LEU:C	2.35	0.52
1:C:307:THR:HG23	1:C:318:GLN:HG2	1.90	0.52
1:A:7:ILE:CG2	1:A:622:LEU:HD22	2.39	0.52
1:C:151:ILE:CG2	2:D:1297:LEU:HD13	2.34	0.52
2:B:898:PHE:HB2	4:F:98:TYR:HA	1.91	0.52
2:D:940:ILE:HG21	2:D:1322:VAL:HG21	1.91	0.52
1:A:108:LEU:HD21	1:A:129:THR:HG22	1.92	0.52
2:D:1514:ALA:HB2	2:D:1583:TRP:CZ2	2.45	0.52
4:H:178:LEU:HD12	4:H:178:LEU:C	2.35	0.52
1:A:213:ILE:HG22	1:A:215:GLU:HG3	1.92	0.52
4:F:159:LEU:HD21	4:F:182:VAL:HG21	1.91	0.52
1:C:346:MET:HE1	1:C:435:HIS:CD2	2.45	0.52
1:A:547:GLN:O	1:A:549:GLU:N	2.43	0.52
2:B:925:LEU:HD13	2:B:1272:LEU:HD13	1.91	0.52
2:B:978:LEU:HB3	2:B:981:LEU:HD12	1.90	0.52
2:B:1272:LEU:HB2	2:B:1289:ILE:HD12	1.91	0.52
2:D:831:ASN:OD1	2:D:833:ARG:HB2	2.10	0.52
2:D:1119:MET:HE2	2:D:1161:LEU:HD11	1.92	0.52
4:H:63:VAL:CG2	4:H:67:PHE:CD2	2.93	0.52
2:B:1035:LEU:HD21	2:B:1077:VAL:HG11	1.91	0.52
2:B:1126:LEU:HA	2:B:1129:LEU:HD12	1.92	0.52
2:D:1147:ILE:HG22	2:D:1177:MET:HE2	1.91	0.52
3:G:37:GLN:HB2	3:G:47:LEU:HD11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1053:SER:HA	2:B:1100:ALA:HB3	1.91	0.51
1:C:210:PHE:CE1	1:C:317:VAL:HG13	2.46	0.51
2:B:1483:LEU:HD13	2:B:1565:PRO:HG3	1.92	0.51
1:A:472:ILE:HG12	1:A:509:LEU:HD22	1.91	0.51
2:B:1522:VAL:HG22	2:B:1583:TRP:HB3	1.92	0.51
1:A:374:THR:HG22	1:C:448:THR:HB	1.93	0.51
1:C:40:PHE:O	1:C:40:PHE:CG	2.63	0.51
2:D:958:ILE:HD12	2:D:1300:GLU:HB2	1.91	0.51
2:B:811:LEU:HG	2:B:813:LEU:HD13	1.92	0.51
2:B:1280:SER:HB2	2:B:1306:GLU:HG3	1.93	0.51
2:D:956:THR:HA	2:D:1324:THR:HG22	1.92	0.51
2:D:1532:LEU:HD23	2:D:1569:ARG:NH1	2.26	0.51
2:B:960:LEU:HD21	2:B:1320:LEU:HD13	1.91	0.51
2:B:1337:ASN:HD21	2:B:1465:GLU:HG2	1.76	0.51
2:B:1507:LEU:HD11	2:B:1629:ALA:CB	2.41	0.51
3:E:147:GLN:OE1	3:E:154:LEU:HD11	2.11	0.51
1:A:53:VAL:O	1:A:53:VAL:HG23	2.11	0.51
1:A:438:VAL:CG1	1:A:449:LEU:HD11	2.41	0.51
1:A:32:PRO:HA	1:A:53:VAL:HG12	1.92	0.51
1:C:6:ILE:HG22	1:C:22:LEU:HD23	1.91	0.51
1:A:350:LEU:HD13	1:A:400:ILE:HG21	1.93	0.50
1:C:434:LEU:HD13	1:C:468:TYR:CE1	2.46	0.50
1:C:112:THR:HG22	1:C:125:TYR:HB3	1.92	0.50
3:G:90:GLN:NE2	3:G:97:THR:OG1	2.44	0.50
2:B:1522:VAL:HG22	2:B:1583:TRP:CB	2.42	0.50
4:H:108:LEU:HD22	4:H:110:THR:HG22	1.94	0.50
2:D:1027:ILE:HG22	2:D:1071:ILE:HD13	1.94	0.50
1:A:3:MET:HE3	1:A:628:SER:HB2	1.94	0.50
2:B:916:MET:HE2	2:B:916:MET:HA	1.93	0.50
1:C:135:LEU:HD22	2:D:789:ASP:O	2.12	0.49
2:D:872:LEU:HD11	2:D:1418:ASP:CG	2.37	0.49
2:D:1147:ILE:HG23	2:D:1177:MET:HE2	1.94	0.49
1:A:249:VAL:HG21	1:A:278:VAL:CG1	2.36	0.49
1:A:374:THR:O	1:A:376:GLN:N	2.46	0.49
2:D:783:LEU:HD12	2:D:784:ALA:N	2.27	0.49
2:D:1527:LEU:HD21	2:D:1530:VAL:CG2	2.42	0.49
3:G:136:LEU:N	3:G:136:LEU:HD12	2.27	0.49
2:D:742:ARG:N	2:D:902:GLY:O	2.44	0.49
1:A:264:GLU:HB3	1:A:284:VAL:HG13	1.93	0.49
1:A:443:LEU:HD11	1:A:449:LEU:HD22	1.93	0.49
3:E:92:TYR:O	3:E:93:ALA:CB	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1539:TYR:CD1	2:B:1574:LEU:HD12	2.48	0.49
3:G:112:ALA:HB1	3:G:201:LEU:CD1	2.39	0.49
4:H:195:ILE:HG22	4:H:210:LYS:HA	1.93	0.49
2:B:1012:TRP:HB3	2:B:1017:LEU:HD12	1.95	0.49
2:D:1119:MET:HG3	2:D:1161:LEU:HD21	1.94	0.49
4:F:12:VAL:HG21	4:F:82(C):LEU:HD13	1.94	0.49
2:B:1068:VAL:HG23	2:B:1069:ASN:ND2	2.27	0.49
2:B:925:LEU:HD22	2:B:1312:ALA:CB	2.41	0.49
4:H:82:MET:HE2	4:H:82(C):LEU:CD2	2.27	0.49
2:B:945:LEU:HD12	2:B:1305:ASN:CG	2.38	0.48
2:B:981:LEU:O	2:B:983:VAL:HG23	2.13	0.48
3:E:22:THR:HG22	3:E:72:THR:HG22	1.95	0.48
1:A:459:ARG:CD	1:C:458:ASP:HB3	2.43	0.48
2:D:1583:TRP:HB2	2:D:1605:TRP:H	1.78	0.48
1:A:452:ASN:HB3	1:A:492:LEU:HD21	1.96	0.48
2:D:1450:ILE:HD11	2:D:1473:PRO:CD	2.42	0.48
2:D:1527:LEU:HD22	2:D:1574:LEU:HB3	1.95	0.48
4:F:116:THR:HG23	4:F:203:SER:HB3	1.95	0.48
3:G:154:LEU:HD23	3:G:155:GLN:N	2.29	0.48
1:C:14:LEU:HD11	1:C:103:LEU:HD12	1.94	0.48
1:C:137:VAL:HG21	1:C:139:ARG:NH1	2.27	0.48
1:C:243:VAL:HG13	1:C:310:LEU:HD22	1.95	0.48
4:H:63:VAL:HG13	4:H:67:PHE:HB2	1.95	0.48
1:A:164:LEU:O	2:B:787:MET:HG2	2.13	0.48
2:D:877:VAL:HG22	2:D:1451:GLN:NE2	2.28	0.48
4:F:178:LEU:C	4:F:178:LEU:HD12	2.37	0.48
1:A:6:ILE:HB	1:A:20:MET:HE3	1.94	0.48
2:B:1133:LYS:NZ	2:B:1147:ILE:HD12	2.28	0.48
1:C:179:MET:HG3	1:C:203:LYS:HA	1.96	0.48
4:F:69:ILE:HA	4:F:79:TYR:O	2.14	0.48
2:B:877:VAL:HG22	2:B:1451:GLN:CG	2.44	0.48
2:B:1143:LEU:HB3	2:B:1144:PRO:HD3	1.95	0.48
1:C:110:ILE:HB	1:C:198:THR:OG1	2.13	0.48
2:D:1141:ASN:O	2:D:1142:SER:CB	2.62	0.48
2:D:1543:ILE:HD13	2:D:1554:VAL:HG11	1.96	0.48
3:E:3:GLN:HE21	3:E:3:GLN:CA	2.26	0.48
1:C:7:ILE:N	1:C:7:ILE:HD12	2.29	0.48
1:C:118:THR:HG23	1:C:205:TYR:CE2	2.49	0.48
2:B:807:PHE:CE1	2:B:840:VAL:HG21	2.49	0.48
2:D:833:ARG:HH11	2:D:836:GLN:NE2	2.12	0.48
2:D:835:ASN:HB2	4:H:54:ASN:ND2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:51:ILE:O	4:F:52(A):PRO:HD3	2.13	0.48
2:D:1274:VAL:HG12	2:D:1276:LEU:CD1	2.44	0.47
1:C:6:ILE:HG21	1:C:20:MET:CE	2.44	0.47
3:E:147:GLN:CD	3:E:154:LEU:HD11	2.39	0.47
1:A:157:SER:O	1:A:158:LEU:HD13	2.14	0.47
1:A:549:GLU:O	1:A:550:ASP:C	2.58	0.47
1:C:459:ARG:HG3	1:C:460:ALA:N	2.29	0.47
2:D:927:PRO:O	2:D:928:GLU:HB2	2.14	0.47
1:A:541:LEU:HD22	2:B:786:SER:HB3	1.96	0.47
2:B:949:VAL:HG13	2:B:950:PRO:HD2	1.95	0.47
2:B:1525:THR:HB	2:B:1541:MET:HE3	1.94	0.47
2:D:1366:ILE:HD13	2:D:1455:VAL:HG11	1.95	0.47
4:F:3:GLN:C	4:F:4:LEU:HD12	2.39	0.47
3:E:11:LEU:HD12	3:E:11:LEU:C	2.40	0.47
3:E:108:ARG:HD3	3:E:109:THR:O	2.14	0.47
3:G:137:ASN:HD21	4:H:183:THR:CG2	2.26	0.47
2:B:877:VAL:HG22	2:B:1451:GLN:HG3	1.96	0.47
1:C:281:SER:OG	1:C:284:VAL:HG23	2.15	0.47
2:D:1161:LEU:HD22	2:D:1166:THR:HG21	1.97	0.47
2:D:1407:ILE:HG22	2:D:1412:LEU:HD13	1.96	0.47
3:E:35:TRP:CE3	3:E:73:LEU:HD12	2.49	0.47
3:G:19:VAL:CG2	3:G:78:LEU:HD22	2.45	0.47
2:B:1107:MET:O	2:B:1248:GLN:HG2	2.14	0.47
2:D:1143:LEU:HB3	2:D:1144:PRO:HD3	1.96	0.47
3:G:137:ASN:ND2	4:H:183:THR:HG21	2.27	0.47
1:A:214:VAL:HG13	1:A:233:ILE:CD1	2.44	0.47
1:A:217:THR:HG23	1:A:230:GLU:O	2.15	0.47
1:A:251:PHE:CD1	1:A:304:VAL:HG22	2.48	0.47
2:B:1024:LEU:HD11	2:B:1070:LEU:HB3	1.96	0.47
2:D:960:LEU:CD2	2:D:1320:LEU:HD13	2.45	0.47
4:F:12:VAL:HG21	4:F:82(C):LEU:CD1	2.45	0.47
3:G:135:LEU:HD22	3:G:136:LEU:N	2.29	0.47
3:G:175:LEU:HD23	3:G:176:SER:N	2.30	0.47
1:A:291:ASN:N	1:A:291:ASN:OD1	2.47	0.47
1:A:363:TYR:CD1	1:A:364:ARG:HG2	2.50	0.47
1:A:541:LEU:HG	2:B:796:ALA:HB2	1.96	0.47
2:B:1163:ARG:O	2:B:1167:VAL:HG23	2.14	0.47
2:B:1385:MET:HE2	2:B:1385:MET:HA	1.97	0.47
2:B:1530:VAL:HG12	2:B:1532:LEU:CD1	2.45	0.47
2:B:1631:THR:O	2:B:1635:VAL:HG23	2.14	0.47
1:C:455:LEU:HD12	1:C:456:ARG:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:960:LEU:HD23	2:D:1320:LEU:HD13	1.97	0.46
2:B:1009:THR:HB	2:B:1011:GLN:HE21	1.79	0.46
2:B:1095:VAL:HG22	2:B:1153:PHE:CE2	2.50	0.46
2:B:1370:TYR:CG	2:B:1376:ALA:HB2	2.51	0.46
1:A:346:MET:HE3	1:A:454:LEU:CD2	2.41	0.46
2:B:1380:ILE:N	2:B:1380:ILE:HD12	2.31	0.46
3:E:191:VAL:HG22	3:E:210:ASN:OD1	2.15	0.46
1:A:346:MET:HE1	1:A:435:HIS:CG	2.50	0.46
2:B:972:ALA:HB1	2:B:1005:TYR:OH	2.15	0.46
2:B:1004:HIS:HB2	2:B:1066:LEU:HD21	1.98	0.46
2:B:1297:LEU:HD23	2:B:1298:ARG:N	2.30	0.46
2:D:1055:TRP:CD2	2:D:1108:ILE:HG22	2.51	0.46
1:A:268:ARG:HB2	2:B:1378:MET:CE	2.39	0.46
4:F:63:VAL:CG2	4:F:67:PHE:CD2	2.99	0.46
2:B:1082:VAL:HG13	2:B:1129:LEU:HD23	1.98	0.46
1:C:214:VAL:HG23	1:C:321:ARG:HB2	1.98	0.46
1:C:408:GLU:C	1:C:409:LEU:HD12	2.41	0.46
1:A:37:VAL:O	1:A:46:VAL:HG13	2.16	0.46
2:B:1375:ASP:OD1	2:B:1430:SER:HB2	2.16	0.46
1:A:548:SER:O	1:A:549:GLU:O	2.34	0.46
2:B:1525:THR:CB	2:B:1541:MET:HE3	2.45	0.46
2:D:835:ASN:HB3	4:H:54:ASN:ND2	2.30	0.46
2:D:1500:LYS:HG2	2:D:1503:ASP:HB2	1.98	0.46
2:D:1530:VAL:HG23	2:D:1576:GLU:HG2	1.98	0.46
1:A:223:ILE:HD13	1:A:298:VAL:CG2	2.46	0.45
2:D:778:THR:OG1	2:D:779:THR:N	2.49	0.45
2:D:872:LEU:HD23	2:D:873:SER:N	2.31	0.45
3:G:29:VAL:HG13	3:G:92:TYR:CB	2.42	0.45
1:C:471:LEU:HD12	1:C:471:LEU:N	2.32	0.45
1:C:495:LEU:HD12	1:C:496:PRO:HD2	1.97	0.45
2:D:1204:GLN:HA	2:D:1207:ASN:ND2	2.31	0.45
1:A:47:LEU:HD23	1:A:47:LEU:O	2.17	0.45
2:B:1582:MET:HE3	2:B:1606:VAL:HB	1.97	0.45
2:D:1045:ALA:HB2	2:D:1052:PRO:HA	1.97	0.45
2:D:1540:ILE:N	2:D:1540:ILE:HD12	2.31	0.45
3:G:163:VAL:HG12	3:G:164:THR:O	2.16	0.45
1:C:210:PHE:CZ	1:C:317:VAL:HG12	2.51	0.45
2:D:1126:LEU:HD11	2:D:1177:MET:CE	2.46	0.45
2:D:1133:LYS:HA	2:D:1143:LEU:HD21	1.98	0.45
4:H:119:PRO:HB2	4:H:142:VAL:HG13	1.97	0.45
1:C:335:PHE:CD2	1:C:419:MET:HB3	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:147:PRO:O	4:H:200:HIS:HE1	2.00	0.45
2:B:1086:ILE:HD12	2:B:1140:VAL:HG11	1.99	0.45
1:C:628:SER:HB2	1:C:630:GLN:OE1	2.17	0.45
4:H:30:THR:O	4:H:30:THR:HG22	2.17	0.45
1:A:590:THR:HG22	1:A:592:SER:H	1.80	0.45
1:A:459:ARG:CZ	1:C:458:ASP:HB2	2.47	0.45
2:B:852:SER:HB3	2:B:878:ILE:HG22	1.98	0.45
2:B:1521:TYR:O	2:B:1583:TRP:HB2	2.16	0.45
2:D:1582:MET:HA	2:D:1605:TRP:O	2.16	0.45
1:A:267:LYS:HG3	1:A:278:VAL:HG23	1.99	0.45
1:A:350:LEU:CD2	1:A:352:VAL:HG22	2.46	0.45
1:A:426:THR:HG21	1:A:431:ASN:HA	1.99	0.45
2:B:809:ILE:HD13	2:B:890:VAL:HG23	1.99	0.45
2:D:920:VAL:HG11	2:D:941:PRO:O	2.16	0.45
4:F:30:THR:HG23	4:F:53:TYR:HA	1.98	0.45
1:C:348:PHE:HE2	1:C:350:LEU:HD12	1.79	0.45
3:G:135:LEU:C	3:G:136:LEU:HD12	2.42	0.45
1:A:487:GLU:H	1:A:490:GLN:HE21	1.65	0.44
2:B:996:MET:HE3	2:B:1027:ILE:HG23	1.99	0.44
2:B:1348:ALA:HB1	2:B:1349:PRO:CD	2.47	0.44
2:D:759:PRO:HA	2:D:760:PRO:HD3	1.85	0.44
2:B:1582:MET:HA	2:B:1605:TRP:O	2.17	0.44
2:D:1496:CYS:O	2:D:1600:ILE:HG22	2.17	0.44
4:F:114:ALA:HB3	4:F:146:PHE:CE1	2.52	0.44
2:B:734:ILE:HD12	2:B:900:SER:HB3	1.98	0.44
1:C:31:VAL:HG13	1:C:54:LEU:HB2	2.00	0.44
1:A:350:LEU:HD12	1:A:400:ILE:CD1	2.47	0.44
2:B:925:LEU:CD1	2:B:1272:LEU:HD13	2.48	0.44
1:C:455:LEU:HD11	1:C:457:MET:HG2	1.99	0.44
2:D:1369:ARG:HD3	2:D:1433:GLU:O	2.17	0.44
4:H:67:PHE:CZ	4:H:82:MET:HE3	2.53	0.44
2:B:1260:TYR:O	2:B:1264:ALA:HB2	2.18	0.44
2:D:1083:LYS:HG3	2:D:1140:VAL:HG13	1.99	0.44
1:A:10:ASN:ND2	1:A:622:LEU:C	2.76	0.44
1:A:375:VAL:O	1:A:375:VAL:HG12	2.18	0.44
2:B:1369:ARG:HD2	2:B:1433:GLU:C	2.43	0.44
1:C:20:MET:CE	1:C:88:ALA:HB2	2.48	0.44
1:C:253:ILE:HD12	1:C:253:ILE:N	2.33	0.44
1:C:352:VAL:HG21	1:C:402:VAL:HG11	2.00	0.44
1:C:453:PHE:HB2	1:C:493:VAL:HG23	2.00	0.44
1:A:510:VAL:HG22	1:A:528:SER:CB	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1061:VAL:HG13	2:B:1078:LEU:HD11	2.00	0.43
1:A:386:LYS:O	1:A:387:LEU:HD23	2.18	0.43
2:B:1253:VAL:HG13	2:B:1254:PHE:CD2	2.53	0.43
1:C:111:GLN:NE2	1:C:574:VAL:HG11	2.33	0.43
3:E:170:ASP:O	3:E:172:THR:HG23	2.18	0.43
3:G:108:ARG:NH1	3:G:111:ALA:HB2	2.33	0.43
2:B:1527:LEU:HD12	2:B:1540:ILE:O	2.18	0.43
2:D:1043:ALA:HB2	2:D:1084:TRP:CD2	2.54	0.43
2:D:1091:LYS:HE3	2:D:1097:GLN:OE1	2.19	0.43
2:B:1527:LEU:HD23	2:B:1575:GLU:O	2.19	0.43
3:G:147:GLN:HG2	3:G:154:LEU:HD21	2.00	0.43
1:C:313:GLY:HA2	2:D:1423:ILE:HD11	2.00	0.43
3:E:21:ILE:HG12	3:E:102:THR:HG21	2.00	0.43
2:B:1091:LYS:HB3	2:B:1092:PRO:HD2	2.01	0.43
2:D:1369:ARG:NH2	2:D:1430:SER:HB3	2.34	0.43
2:B:1520:ASP:O	2:B:1550:GLY:HA3	2.19	0.43
1:C:147:ASN:HB2	1:C:148:PRO:CD	2.48	0.43
1:C:302:LEU:HD21	1:C:326:ILE:HD11	2.01	0.43
2:D:925:LEU:HD23	2:D:936:GLN:NE2	2.33	0.43
4:F:27:PHE:CE2	4:F:94:ARG:HD2	2.53	0.43
3:G:29:VAL:O	3:G:29:VAL:CG1	2.66	0.43
2:D:1413:ASP:O	2:D:1414:LYS:C	2.62	0.43
3:G:136:LEU:N	3:G:136:LEU:CD1	2.82	0.43
1:A:347:PRO:HD3	1:C:492:LEU:HB3	2.00	0.43
2:B:1111:LEU:HD12	2:B:1165:TYR:HE2	1.84	0.43
2:B:1490:ARG:HG2	2:B:1590:TRP:CZ2	2.54	0.43
2:B:1525:THR:OG1	2:B:1541:MET:HE3	2.19	0.43
1:C:291:ASN:ND2	1:C:296:ASP:OD2	2.51	0.43
4:F:94:ARG:O	4:F:100(F):MET:HA	2.19	0.43
4:H:50:LEU:HD12	4:H:50:LEU:C	2.43	0.43
1:A:453:PHE:O	1:A:492:LEU:HD23	2.19	0.42
1:C:573:LEU:HD23	2:D:784:ALA:CB	2.49	0.42
4:H:18:LEU:HD12	4:H:109:VAL:HG13	2.01	0.42
1:A:538:VAL:HG12	2:B:791:LYS:HG2	2.00	0.42
1:C:137:VAL:HG21	1:C:139:ARG:CZ	2.49	0.42
2:D:919:THR:CG2	2:D:922:VAL:HG13	2.49	0.42
3:E:113:PRO:HD3	3:E:198:HIS:CD2	2.53	0.42
3:E:136:LEU:HD12	3:E:136:LEU:N	2.35	0.42
4:F:63:VAL:CG1	4:F:67:PHE:HB2	2.45	0.42
3:G:25:ALA:HB3	3:G:69:THR:HA	1.99	0.42
2:B:914:ILE:HG23	2:B:915:ARG:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:LEU:HG	2:D:1378:MET:HE1	2.01	0.42
2:D:1349:PRO:O	2:D:1350:GLU:C	2.62	0.42
1:C:36:THR:HG22	1:C:87:GLN:O	2.20	0.42
1:C:110:ILE:HD13	1:C:184:ILE:O	2.20	0.42
2:D:960:LEU:O	2:D:1297:LEU:HA	2.19	0.42
2:D:936:GLN:O	2:D:1311:THR:HG23	2.19	0.42
1:A:377:SER:O	1:A:378:LEU:C	2.61	0.42
1:A:445:PRO:HB3	1:A:500:THR:C	2.44	0.42
2:B:1552:ASP:OD1	2:B:1596:LEU:HD13	2.19	0.42
4:F:63:VAL:HG21	4:F:67:PHE:CD2	2.54	0.42
3:G:115:VAL:HG22	3:G:196:VAL:HG21	2.01	0.42
1:A:377:SER:O	1:A:385:ALA:HB1	2.20	0.42
1:A:492:LEU:HB3	1:C:347:PRO:HD3	2.02	0.42
2:B:1547:ILE:HG12	2:B:1631:THR:HG23	2.00	0.42
2:D:1228:PRO:O	2:D:1232:ARG:HB2	2.19	0.42
3:E:150:VAL:HG22	3:E:192:TYR:CD2	2.55	0.42
4:F:75:LYS:O	4:F:76:ASN:C	2.63	0.42
1:A:3:MET:HE3	1:A:522:ARG:HG2	2.02	0.42
1:A:547:GLN:C	1:A:549:GLU:N	2.77	0.42
1:C:50:GLU:HB3	1:C:64:VAL:HG13	2.02	0.42
1:C:251:PHE:CD1	1:C:304:VAL:HG22	2.55	0.42
3:E:31:THR:O	3:E:31:THR:HG23	2.18	0.42
2:B:918:LYS:H	2:B:1323:VAL:HG13	1.85	0.42
1:C:266:LEU:HD21	2:D:1378:MET:HE2	2.01	0.42
2:D:1291:TRP:CD1	2:D:1291:TRP:C	2.98	0.42
1:A:157:SER:C	1:A:158:LEU:HD22	2.45	0.41
2:B:1074:ASP:HB3	2:B:1077:VAL:HG23	2.01	0.41
2:B:1447:VAL:CG1	2:B:1450:ILE:HG22	2.48	0.41
1:A:123:VAL:CG2	1:A:173:ILE:HD11	2.50	0.41
1:A:135:LEU:HD23	2:B:792:GLY:CA	2.49	0.41
1:A:459:ARG:NE	1:C:458:ASP:HB3	2.35	0.41
1:C:589:LEU:HG	2:D:795:VAL:HG21	2.01	0.41
2:D:1543:ILE:HD12	2:D:1554:VAL:CG2	2.49	0.41
1:A:333:ILE:HD11	1:A:404:THR:HG23	2.03	0.41
2:B:1532:LEU:HD12	2:B:1532:LEU:N	2.36	0.41
1:C:114:LYS:NZ	2:D:747:GLU:OE1	2.53	0.41
1:C:455:LEU:HB2	1:C:468:TYR:OH	2.21	0.41
2:D:1008:GLU:CD	2:D:1262:LYS:HG2	2.44	0.41
2:D:1504:LYS:O	2:D:1504:LYS:CG	2.64	0.41
1:A:438:VAL:CG1	1:A:449:LEU:HD21	2.44	0.41
1:C:14:LEU:HD11	1:C:103:LEU:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:SER:C	1:C:158:LEU:HD22	2.46	0.41
2:D:1003:VAL:CG1	2:D:1070:LEU:HD13	2.50	0.41
3:E:182:SER:O	3:E:183:LYS:C	2.63	0.41
1:A:427:VAL:HB	1:A:523:GLU:HG3	2.02	0.41
1:A:547:GLN:O	1:A:548:SER:C	2.63	0.41
2:B:1341:LEU:HD13	2:B:1457:VAL:HG11	2.03	0.41
2:D:783:LEU:HD12	2:D:784:ALA:H	1.85	0.41
2:D:1391:PRO:HB2	2:D:1396:LEU:HD11	2.02	0.41
2:D:1506:THR:N	2:D:1509:GLU:HG3	2.36	0.41
3:E:112:ALA:HB1	3:E:201:LEU:HD13	2.01	0.41
3:G:54:LEU:HD11	3:G:58:VAL:HG11	2.02	0.41
3:G:191:VAL:HG22	3:G:210:ASN:OD1	2.20	0.41
4:H:30:THR:O	4:H:30:THR:CG2	2.68	0.41
2:B:1274:VAL:HG12	2:B:1276:LEU:CD1	2.51	0.41
2:B:1396:LEU:HD12	2:B:1419:ARG:NH1	2.35	0.41
2:D:990:GLU:OE2	2:D:1046:ALA:HB2	2.20	0.41
2:D:1231:VAL:HG21	2:D:1260:TYR:CE1	2.56	0.41
3:E:158:ASN:H	3:E:158:ASN:HD22	1.67	0.41
4:H:63:VAL:HG22	4:H:67:PHE:CD1	2.56	0.41
1:A:344:PRO:HG2	1:A:395:GLN:HE22	1.86	0.41
2:B:1528:VAL:CG2	2:B:1542:ALA:HB2	2.51	0.41
2:D:996:MET:O	2:D:1000:VAL:HG23	2.20	0.41
2:D:1403:VAL:O	2:D:1404:ASP:HB2	2.21	0.41
2:D:1451:GLN:O	2:D:1452:PRO:C	2.64	0.41
3:E:124:GLN:HE22	3:E:131:SER:HB2	1.86	0.41
1:A:83:PHE:CE1	2:B:1017:LEU:HD22	2.56	0.41
2:B:1341:LEU:HD22	2:B:1457:VAL:HG13	2.03	0.41
2:B:1617:ASP:O	2:B:1618:GLU:C	2.64	0.41
1:C:11:ILE:HD11	1:C:635:ARG:CZ	2.50	0.41
1:C:558:GLN:HG3	2:D:772:PHE:CE1	2.56	0.41
2:D:961:GLN:NE2	2:D:963:THR:HG23	2.35	0.41
2:D:1119:MET:CE	2:D:1161:LEU:HD11	2.51	0.41
3:G:39:LYS:NZ	3:G:81:GLU:O	2.48	0.41
1:A:347:PRO:CG	1:C:492:LEU:HD22	2.46	0.41
2:B:858:ARG:CZ	2:B:1449:LEU:HD12	2.51	0.41
2:D:959:LEU:HD23	2:D:959:LEU:C	2.47	0.41
1:A:10:ASN:HB3	1:A:635:ARG:HD3	2.02	0.40
1:A:36:THR:HG23	1:A:48:SER:CB	2.52	0.40
1:A:297:LEU:HB3	1:A:326:ILE:HD13	2.03	0.40
2:B:935:VAL:O	2:B:936:GLN:C	2.64	0.40
2:B:1213:TYR:CD1	2:B:1252:MET:HE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1270:LEU:HD12	2:B:1291:TRP:HB2	2.03	0.40
2:B:1369:ARG:HE	2:B:1430:SER:HB3	1.86	0.40
2:B:1530:VAL:HG12	2:B:1532:LEU:HD12	2.03	0.40
4:F:12:VAL:CG2	4:F:111:VAL:HG22	2.49	0.40
4:F:136:ALA:HB2	4:F:186:SER:HB3	2.04	0.40
1:C:289:VAL:HG12	1:C:291:ASN:HB2	2.03	0.40
3:E:150:VAL:HG13	3:E:192:TYR:CE2	2.56	0.40
2:B:1147:ILE:HG23	2:B:1177:MET:CE	2.51	0.40
1:C:100:LEU:HD12	1:C:101:VAL:H	1.86	0.40
2:D:935:VAL:HG11	2:D:1313:GLU:HG3	2.02	0.40
2:D:1091:LYS:HB3	2:D:1092:PRO:HD2	2.03	0.40
2:D:1278:LEU:HD22	2:D:1302:THR:HG21	2.03	0.40
4:F:17:SER:HB2	4:H:72:ASN:ND2	2.35	0.40
1:A:163:GLN:HE21	1:A:163:GLN:HB2	1.68	0.40
2:B:1172:TYR:CE1	2:B:1216:LEU:HB3	2.56	0.40
2:B:1619:GLU:O	2:B:1620:ASN:CB	2.69	0.40
1:C:510:VAL:HG22	1:C:528:SER:HB3	2.04	0.40
2:D:1172:TYR:CE1	2:D:1216:LEU:HB3	2.57	0.40
2:D:1310:VAL:HG11	2:D:1320:LEU:CD2	2.51	0.40
2:D:1062:LYS:HE3	2:D:1124:PHE:CE1	2.57	0.40
2:D:1274:VAL:HG12	2:D:1276:LEU:HD11	2.03	0.40
3:G:124:GLN:HE21	3:G:129:THR:HG22	1.87	0.40
3:G:147:GLN:CG	3:G:154:LEU:HD11	2.50	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	640/644 (99%)	595 (93%)	37 (6%)	8 (1%)	9	35
1	C	640/644 (99%)	581 (91%)	48 (8%)	11 (2%)	7	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	897/915 (98%)	798 (89%)	79 (9%)	20 (2%)	5	24
2	D	897/915 (98%)	809 (90%)	70 (8%)	18 (2%)	6	25
3	E	212/214 (99%)	204 (96%)	8 (4%)	0	100	100
3	G	212/214 (99%)	200 (94%)	12 (6%)	0	100	100
4	F	217/226 (96%)	203 (94%)	12 (6%)	2 (1%)	14	44
4	H	217/226 (96%)	211 (97%)	6 (3%)	0	100	100
All	All	3932/3998 (98%)	3601 (92%)	272 (7%)	59 (2%)	8	32

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	548	SER
1	A	549	GLU
2	B	913	GLY
2	B	935	VAL
2	B	968	MET
2	B	1497	PHE
1	C	41	PRO
1	C	59	ASN
1	C	292	PRO
1	C	442	GLU
1	C	459	ARG
2	D	1334	LEU
2	D	1360	ASN
2	D	1417	SER
2	D	1476	GLU
2	D	1640	PRO
4	F	98	TYR
1	A	375	VAL
2	B	914	ILE
2	B	1292	GLU
2	B	1429	VAL
2	B	1450	ILE
2	B	1476	GLU
2	B	1478	GLY
2	B	1620	ASN
2	D	928	GLU
2	D	1142	SER
2	D	1292	GLU
2	D	1350	GLU

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Mol	Chain	Res	Type
2	D	1429	VAL
2	D	1432	SER
2	D	1450	ILE
1	A	550	ASP
2	B	911	PRO
2	B	1334	LEU
2	B	1378	MET
2	B	1592	GLU
2	B	1618	GLU
1	C	294	ALA
1	C	518	ALA
2	D	1377	THR
1	A	49	SER
1	A	552	GLN
2	B	1335	THR
1	C	76	SER
1	C	552	GLN
2	D	944	ASP
2	D	1449	LEU
4	F	114	ALA
2	B	1315	LYS
1	C	81	ASN
1	A	91	GLY
2	B	1331	LYS
1	C	291	ASN
2	D	1349	PRO
1	A	517	GLY
2	D	1016	GLY
2	D	1314	GLY
2	B	982	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	566/567 (100%)	525 (93%)	41 (7%)	13 40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	566/567 (100%)	542 (96%)	24 (4%)	26	58
2	B	799/810 (99%)	754 (94%)	45 (6%)	19	49
2	D	799/810 (99%)	751 (94%)	48 (6%)	17	47
3	E	188/188 (100%)	169 (90%)	19 (10%)	7	28
3	G	188/188 (100%)	165 (88%)	23 (12%)	5	20
4	F	181/185 (98%)	160 (88%)	21 (12%)	5	22
4	H	181/185 (98%)	163 (90%)	18 (10%)	7	29
All	All	3468/3500 (99%)	3229 (93%)	239 (7%)	14	41

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	A	31	VAL
1	A	36	THR
1	A	45	LEU
1	A	46	VAL
1	A	51	LYS
1	A	54	LEU
1	A	64	VAL
1	A	71	ASN
1	A	75	LYS
1	A	93	GLN
1	A	104	GLN
1	A	163	GLN
1	A	178	ASN
1	A	215	GLU
1	A	219	LYS
1	A	223	ILE
1	A	243	VAL
1	A	249	VAL
1	A	259	ARG
1	A	260	ILE
1	A	291	ASN
1	A	317	VAL
1	A	332	GLN
1	A	408	GLU
1	A	425	SER
1	A	464	LYS
1	A	466	ARG

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Mol	Chain	Res	Type
1	A	475	LYS
1	A	492	LEU
1	A	509	LEU
1	A	521	GLN
1	A	542	VAL
1	A	551	ARG
1	A	554	VAL
1	A	583	LEU
1	A	596	ASP
1	A	611	LYS
1	A	634	GLN
1	A	639	GLN
1	A	642	GLN
2	B	730	ASP
2	B	743	SER
2	B	758	GLU
2	B	783	LEU
2	B	790	LYS
2	B	813	LEU
2	B	826	ARG
2	B	834	GLN
2	B	835	ASN
2	B	841	ARG
2	B	861	GLN
2	B	883	THR
2	B	890	VAL
2	B	894	VAL
2	B	912	GLU
2	B	914	ILE
2	B	938	GLU
2	B	949	VAL
2	B	968	MET
2	B	1088	GLU
2	B	1106	GLU
2	B	1138	GLU
2	B	1269	GLU
2	B	1325	MET
2	B	1334	LEU
2	B	1369	ARG
2	B	1378	MET
2	B	1387	THR
2	B	1393	THR

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Mol	Chain	Res	Type
2	B	1428	LYS
2	B	1429	VAL
2	B	1431	HIS
2	B	1450	ILE
2	B	1479	LYS
2	B	1490	ARG
2	B	1500	LYS
2	B	1504	LYS
2	B	1537	ASP
2	B	1566	ILE
2	B	1575	GLU
2	B	1590	TRP
2	B	1606	VAL
2	B	1618	GLU
2	B	1620	ASN
2	B	1632	GLU
1	C	31	VAL
1	C	142	MET
1	C	194	GLN
1	C	234	THR
1	C	249	VAL
1	C	277	GLU
1	C	293	ARG
1	C	317	VAL
1	C	320	GLU
1	C	350	LEU
1	C	399	SER
1	C	406	LYS
1	C	437	SER
1	C	444	ARG
1	C	457	MET
1	C	464	LYS
1	C	509	LEU
1	C	554	VAL
1	C	558	GLN
1	C	597	VAL
1	C	625	THR
1	C	628	SER
1	C	634	GLN
1	C	639	GLN
2	D	789	ASP
2	D	804	MET

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Mol	Chain	Res	Type
2	D	826	ARG
2	D	833	ARG
2	D	841	ARG
2	D	861	GLN
2	D	882	LYS
2	D	890	VAL
2	D	894	VAL
2	D	968	MET
2	D	984	THR
2	D	1017	LEU
2	D	1018	GLU
2	D	1024	LEU
2	D	1050	ARG
2	D	1141	ASN
2	D	1149	LYS
2	D	1181	LYS
2	D	1204	GLN
2	D	1288	ARG
2	D	1325	MET
2	D	1346	LYS
2	D	1369	ARG
2	D	1378	MET
2	D	1393	THR
2	D	1412	LEU
2	D	1429	VAL
2	D	1431	HIS
2	D	1445	PHE
2	D	1450	ILE
2	D	1462	ASN
2	D	1487	GLU
2	D	1488	LEU
2	D	1490	ARG
2	D	1499	GLN
2	D	1500	LYS
2	D	1503	ASP
2	D	1504	LYS
2	D	1506	THR
2	D	1507	LEU
2	D	1509	GLU
2	D	1548	LYS
2	D	1566	ILE
2	D	1583	TRP

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Mol	Chain	Res	Type
2	D	1605	TRP
2	D	1606	VAL
2	D	1625	GLN
2	D	1641	ASN
3	E	1	ASP
3	E	3	GLN
3	E	19	VAL
3	E	31	THR
3	E	63	SER
3	E	73	LEU
3	E	88	CYS
3	E	89	GLN
3	E	90	GLN
3	E	94	THR
3	E	100	GLN
3	E	103	LYS
3	E	108	ARG
3	E	135	LEU
3	E	158	ASN
3	E	164	THR
3	E	187	GLU
3	E	197	THR
3	E	201	LEU
4	F	11	LEU
4	F	12	VAL
4	F	18	LEU
4	F	32	SER
4	F	63	VAL
4	F	68	THR
4	F	75	LYS
4	F	100	SER
4	F	100(C)	TYR
4	F	100(D)	TYR
4	F	100(F)	MET
4	F	105	GLN
4	F	107	THR
4	F	108	LEU
4	F	110	THR
4	F	116	THR
4	F	117	LYS
4	F	140	CYS
4	F	170	LEU

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Mol	Chain	Res	Type
4	F	183	THR
4	F	206	LYS
3	G	3	GLN
3	G	12	SER
3	G	18	ARG
3	G	20	THR
3	G	23	CYS
3	G	31	THR
3	G	39	LYS
3	G	45	LYS
3	G	73	LEU
3	G	88	CYS
3	G	90	GLN
3	G	91	SER
3	G	108	ARG
3	G	125	LEU
3	G	129	THR
3	G	135	LEU
3	G	145	LYS
3	G	149	LYS
3	G	158	ASN
3	G	164	THR
3	G	165	GLU
3	G	176	SER
3	G	201	LEU
4	H	7	SER
4	H	11	LEU
4	H	12	VAL
4	H	18	LEU
4	H	28	SER
4	H	34	VAL
4	H	63	VAL
4	H	72	ASN
4	H	85	GLU
4	H	105	GLN
4	H	108	LEU
4	H	110	THR
4	H	117	LYS
4	H	160	THR
4	H	170	LEU
4	H	172	SER
4	H	186	SER

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Mol	Chain	Res	Type
4	H	189	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	28	GLN
1	A	81	ASN
1	A	104	GLN
1	A	155	GLN
1	A	162	ASN
1	A	163	GLN
1	A	178	ASN
1	A	194	GLN
1	A	254	GLN
1	A	332	GLN
1	A	334	HIS
1	A	376	GLN
1	A	395	GLN
1	A	490	GLN
1	A	547	GLN
1	A	552	GLN
1	A	558	GLN
1	A	634	GLN
2	B	805	GLN
2	B	836	GLN
2	B	961	GLN
2	B	1069	ASN
2	B	1090	GLN
2	B	1113	ASN
2	B	1115	ASN
2	B	1130	GLN
2	B	1141	ASN
2	B	1160	ASN
2	B	1204	GLN
2	B	1259	GLN
2	B	1277	GLN
2	B	1317	GLN
2	B	1360	ASN
2	B	1401	ASN
2	B	1443	GLN
2	B	1451	GLN

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Mol	Chain	Res	Type
2	B	1462	ASN
2	B	1481	ASN
2	B	1499	GLN
2	B	1531	GLN
2	B	1559	GLN
2	B	1620	ASN
1	C	10	ASN
1	C	81	ASN
1	C	111	GLN
1	C	132	HIS
1	C	155	GLN
1	C	163	GLN
1	C	190	ASN
1	C	254	GLN
1	C	318	GLN
1	C	370	GLN
1	C	435	HIS
1	C	587	ASN
1	C	639	GLN
2	D	805	GLN
2	D	834	GLN
2	D	835	ASN
2	D	836	GLN
2	D	961	GLN
2	D	1130	GLN
2	D	1186	ASN
2	D	1204	GLN
2	D	1277	GLN
2	D	1327	HIS
2	D	1333	GLN
2	D	1360	ASN
2	D	1401	ASN
2	D	1443	GLN
2	D	1451	GLN
2	D	1481	ASN
3	E	3	GLN
3	E	37	GLN
3	E	79	GLN
3	E	89	GLN
3	E	100	GLN
3	E	124	GLN
3	E	138	ASN

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Mol	Chain	Res	Type
3	E	158	ASN
3	E	199	GLN
4	F	57	ASN
4	F	76	ASN
4	F	105	GLN
4	F	164	HIS
4	F	200	HIS
3	G	3	GLN
3	G	79	GLN
3	G	90	GLN
3	G	137	ASN
3	G	147	GLN
3	G	158	ASN
3	G	160	GLN
3	G	199	GLN
4	H	54	ASN
4	H	72	ASN
4	H	95	ASN
4	H	105	GLN
4	H	192	GLN
4	H	200	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 2 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	642/644 (99%)	-0.24	9 (1%) 73 53	3, 29, 61, 99	0
1	C	642/644 (99%)	-0.18	8 (1%) 76 58	3, 31, 64, 119	0
2	B	903/915 (98%)	0.75	148 (16%) 4 2	2, 72, 148, 165	0
2	D	903/915 (98%)	0.09	76 (8%) 17 9	2, 26, 144, 154	0
3	E	214/214 (100%)	-0.33	0 100 100	4, 24, 47, 82	0
3	G	214/214 (100%)	-0.31	1 (0%) 87 73	2, 13, 43, 77	0
4	F	221/226 (97%)	-0.42	0 100 100	2, 18, 58, 91	0
4	H	221/226 (97%)	-0.46	1 (0%) 87 73	2, 12, 36, 86	0
All	All	3960/3998 (99%)	0.04	243 (6%) 27 15	2, 29, 133, 165	0

All (243) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1324	THR	6.4
2	B	1300	GLU	5.8
2	D	1294	ALA	5.6
2	D	1295	SER	4.9
2	B	1272	LEU	4.8
2	B	1274	VAL	4.8
2	D	925	LEU	4.6
2	B	1327	HIS	4.6
2	D	1318	GLY	4.6
2	D	921	ALA	4.5
2	B	1325	MET	4.5
2	D	920	VAL	4.5
2	D	951	ASP	4.4
2	B	1315	LYS	4.4
2	B	1282	SER	4.3
2	D	924	THR	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	48	SER	4.1
2	D	926	ASP	4.1
2	B	1203	LYS	4.0
2	B	1096	PHE	4.0
2	D	1321	SER	4.0
2	B	937	LYS	4.0
2	D	945	LEU	4.0
2	B	949	VAL	3.9
2	B	1265	PRO	3.9
2	B	943	ALA	3.9
2	D	946	SER	3.9
2	B	1206	TYR	3.9
2	B	1267	HIS	3.8
2	B	950	PRO	3.8
2	B	1278	LEU	3.8
2	B	1326	TYR	3.8
2	B	1135	ILE	3.8
2	D	1316	GLY	3.8
2	B	1115	ASN	3.8
2	B	1430	SER	3.7
2	B	1270	LEU	3.7
2	D	1285	ILE	3.7
2	D	1306	GLU	3.6
2	D	966	ALA	3.6
2	D	1327	HIS	3.6
2	B	924	THR	3.6
2	B	930	LEU	3.6
2	D	918	LYS	3.6
2	B	1323	VAL	3.6
2	B	1092	PRO	3.6
2	B	965	VAL	3.5
2	B	1201	PRO	3.5
2	B	1289	ILE	3.5
1	A	48	SER	3.5
2	B	1321	SER	3.5
1	A	76	SER	3.4
2	B	1320	LEU	3.4
2	B	942	PRO	3.4
2	B	1243	GLY	3.4
1	A	375	VAL	3.4
2	B	1116	GLU	3.4
1	A	371	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
2	D	1416	PHE	3.3
2	B	1293	SER	3.3
2	B	1120	ALA	3.3
2	B	1184	LEU	3.3
2	B	1140	VAL	3.3
2	D	1328	ALA	3.3
2	B	941	PRO	3.3
2	B	1101	PRO	3.3
1	C	375	VAL	3.3
2	B	1205	LEU	3.3
2	D	919	THR	3.2
2	B	1196	ASN	3.2
2	D	1270	LEU	3.2
2	D	956	THR	3.2
2	D	963	THR	3.2
2	B	1314	GLY	3.2
2	B	1431	HIS	3.2
2	B	1590	TRP	3.2
1	C	76	SER	3.2
2	D	1282	SER	3.2
2	B	952	THR	3.2
1	C	374	THR	3.1
2	B	954	SER	3.1
2	D	930	LEU	3.1
2	D	1324	THR	3.1
2	B	1268	GLN	3.1
2	D	1326	TYR	3.1
2	B	1083	LYS	3.1
2	B	927	PRO	3.1
2	D	1297	LEU	3.0
2	B	948	GLN	3.0
2	D	1605	TRP	3.0
2	B	1121	LEU	3.0
2	D	917	ASN	3.0
2	D	1323	VAL	3.0
2	B	1053	SER	3.0
2	D	1329	LYS	3.0
4	H	216	CYS	3.0
2	B	1294	ALA	3.0
2	D	1319	THR	2.9
2	D	922	VAL	2.9
2	B	944	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	940	ILE	2.9
2	B	919	THR	2.9
2	B	1312	ALA	2.9
2	B	1245	GLY	2.9
2	D	1320	LEU	2.9
2	D	950	PRO	2.9
2	B	925	LEU	2.9
2	B	1263	ASP	2.8
2	B	956	THR	2.8
2	D	935	VAL	2.8
2	D	1291	TRP	2.8
2	D	1280	SER	2.8
2	B	957	ARG	2.8
2	B	945	LEU	2.8
2	B	958	ILE	2.8
2	B	1285	ILE	2.8
2	B	1093	ASP	2.8
2	B	1291	TRP	2.8
2	D	1325	MET	2.8
2	B	1273	ASP	2.8
2	B	1078	LEU	2.8
2	D	943	ALA	2.7
2	B	1166	THR	2.7
2	B	1239	TYR	2.7
1	A	518	ALA	2.7
2	D	1417	SER	2.7
2	B	917	ASN	2.7
2	B	1117	LYS	2.7
2	D	1430	SER	2.7
2	B	1158	TYR	2.7
2	D	937	LYS	2.6
2	B	1168	ALA	2.6
2	D	1312	ALA	2.6
2	B	1044	PHE	2.6
2	B	1290	HIS	2.6
2	B	938	GLU	2.6
2	B	1095	VAL	2.6
2	B	1322	VAL	2.6
1	C	440	ARG	2.6
2	B	1351	THR	2.6
2	B	1202	GLY	2.6
2	B	1369	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	1026	LEU	2.5
2	B	1142	SER	2.5
2	B	1149	LYS	2.5
2	D	1639	CYS	2.5
2	B	1415	ALA	2.5
2	B	1104	HIS	2.5
2	D	1276	LEU	2.5
2	D	934	GLY	2.5
2	D	1372	GLY	2.5
2	D	1304	GLU	2.5
2	D	1283	SER	2.4
2	D	1289	ILE	2.4
2	B	953	GLU	2.4
2	B	1069	ASN	2.4
2	B	1292	GLU	2.4
2	B	960	LEU	2.4
2	D	1265	PRO	2.4
2	B	1281	ARG	2.4
2	B	946	SER	2.4
2	D	1293	SER	2.4
1	A	458	ASP	2.4
2	D	1431	HIS	2.4
2	B	936	GLN	2.4
2	D	1317	GLN	2.4
1	C	74	PHE	2.4
2	B	922	VAL	2.4
2	D	941	PRO	2.4
2	D	1310	VAL	2.4
2	D	923	ARG	2.4
2	B	1090	GLN	2.4
2	B	1037	PHE	2.4
2	B	1308	PHE	2.4
2	B	1180	LEU	2.4
2	B	1337	ASN	2.3
2	B	1373	ASP	2.3
3	G	154	LEU	2.3
2	D	1322	VAL	2.3
1	C	41	PRO	2.3
2	B	1183	PRO	2.3
2	B	1148	THR	2.3
2	B	1302	THR	2.3
2	D	1315	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	968	MET	2.3
1	A	75	LYS	2.3
2	B	962	GLY	2.3
2	B	1046	ALA	2.3
2	B	1199	GLU	2.3
2	B	1191	THR	2.3
2	D	944	ASP	2.3
2	D	916	MET	2.3
2	D	960	LEU	2.3
1	C	75	LYS	2.3
2	B	967	GLN	2.3
2	D	952	THR	2.2
2	B	1313	GLU	2.2
2	B	1103	ILE	2.2
2	D	929	ARG	2.2
2	B	935	VAL	2.2
2	D	1401	ASN	2.2
2	B	951	ASP	2.2
2	B	1040	PRO	2.2
2	B	1287	HIS	2.2
2	D	936	GLN	2.2
2	B	1235	ASN	2.2
2	D	1284	LYS	2.2
2	B	1296	LEU	2.2
1	A	374	THR	2.1
2	B	1244	TYR	2.1
2	B	1147	ILE	2.1
2	B	1023	ALA	2.1
2	B	1316	GLY	2.1
2	D	1307	GLY	2.1
2	B	1331	LYS	2.1
2	B	995	GLY	2.1
2	B	1594	PRO	2.1
2	B	939	ASP	2.1
2	B	1198	TRP	2.1
2	B	1221	LEU	2.1
2	B	1334	LEU	2.1
2	D	1272	LEU	2.1
2	D	1286	THR	2.1
2	B	1144	PRO	2.1
1	A	377	SER	2.1
2	B	1195	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	1593	LYS	2.1
2	B	1027	ILE	2.1
2	B	1159	MET	2.1
2	B	1256	ALA	2.1
2	D	964	PRO	2.1
2	D	1308	PHE	2.1
2	D	1487	GLU	2.1
2	B	1086	ILE	2.1
2	B	1288	ARG	2.1
2	B	1266	ASP	2.1
2	B	1181	LYS	2.0
2	B	959	LEU	2.0
2	B	1276	LEU	2.0
2	B	934	GLY	2.0
2	B	1111	LEU	2.0
2	B	1284	LYS	2.0
2	B	1024	LEU	2.0

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

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

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($\text{\AA}^2$)	Q<0.9
5	CA	C	645	1/1	0.95	0.05	54,54,54,54	0
5	CA	A	645	1/1	0.96	0.03	47,47,47,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.