



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:42 PM GMT

PDB ID : 3M1B
Title : Crystal structure of human FcRn with a dimeric peptide inhibitor
Authors : Mezo, A.R.; Sridhar, V.; Badger, J.; Sakorafas, P.; Nienaber, V.
Deposited on : 2010-03-04
Resolution : 3.10 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

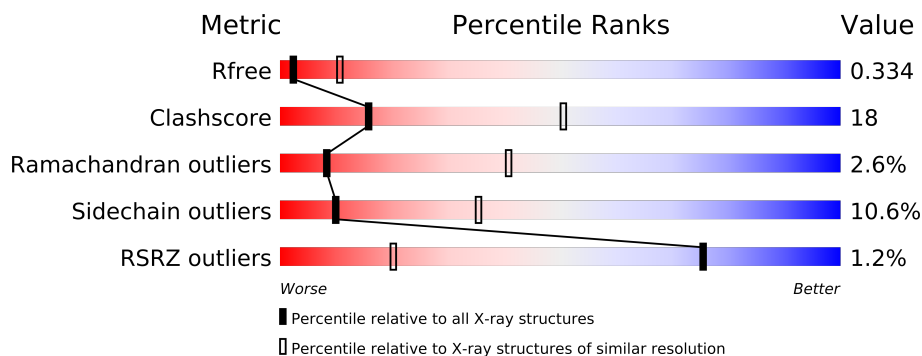
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 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}	66092	1007 (3.18-3.02)
Clashscore	79885	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RSRZ outliers	66119	1008 (3.18-3.02)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	267	
1	C	267	
1	E	267	
1	G	267	
2	B	99	
2	D	99	
2	F	99	
2	H	99	
3	I	16	
3	J	16	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11241 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called IgG receptor FcRn large subunit p51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			1958	1253	329	368	8			
1	C	263	Total	C	N	O	S	0	0	0
			1958	1253	329	368	8			
1	E	263	Total	C	N	O	S	0	0	0
			1958	1253	329	368	8			
1	G	263	Total	C	N	O	S	0	0	0
			1958	1253	329	368	8			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			808	514	135	156	3			
2	D	99	Total	C	N	O	S	0	0	0
			808	514	135	156	3			
2	F	99	Total	C	N	O	S	0	0	0
			808	514	135	156	3			
2	H	99	Total	C	N	O	S	0	0	0
			808	514	135	156	3			

- Molecule 3 is a protein called DIMERIC PEPTIDE INHIBITOR.

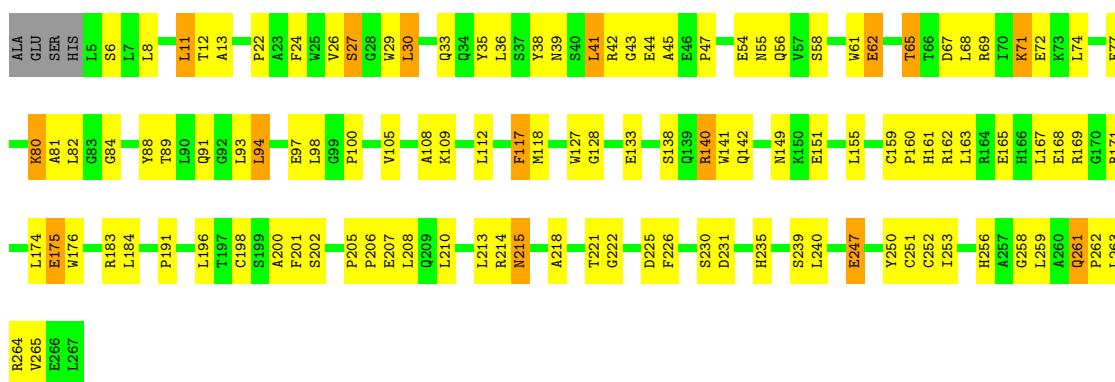
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	11	Total	C	N	O	S	0	0	0
			83	55	13	13	2			
3	J	12	Total	C	N	O	S	0	0	0
			94	64	14	14	2			

3 Residue-property plots

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

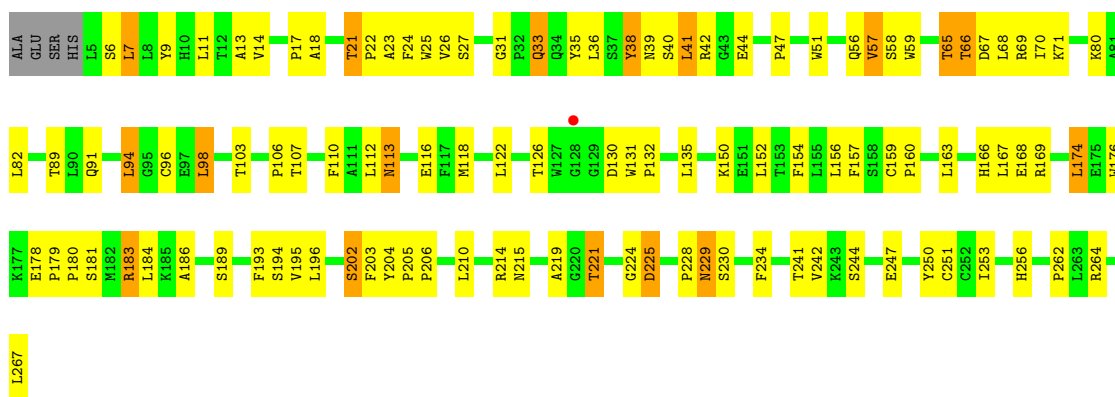
• Molecule 1: IgG receptor FcRn large subunit p51

Chain A:



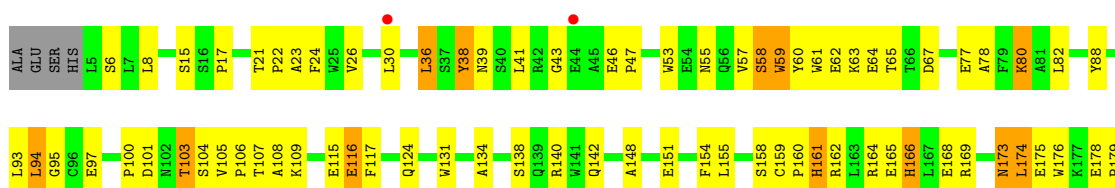
• Molecule 1: IgG receptor FcRn large subunit p51

Chain C:



• Molecule 1: IgG receptor FcRn large subunit p51

Chain E:





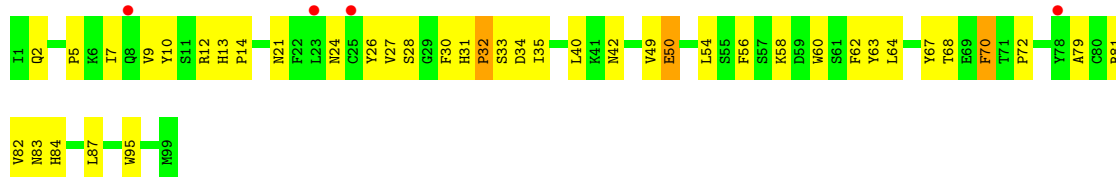
- Molecule 1: IgG receptor FcRn large subunit p51

Chain G:



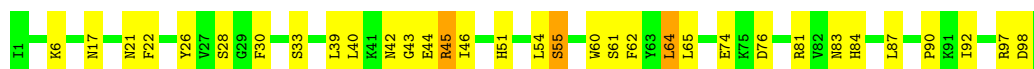
- Molecule 2: Beta-2-microglobulin

Chain B:



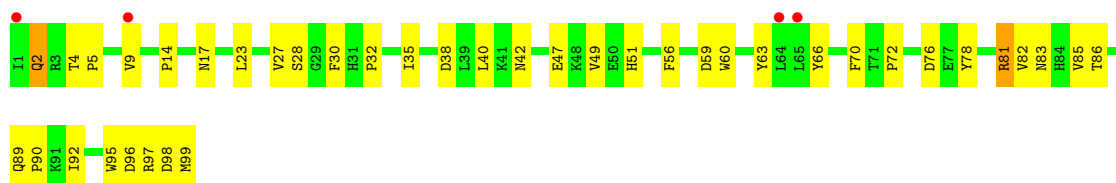
- Molecule 2: Beta-2-microglobulin

Chain D:



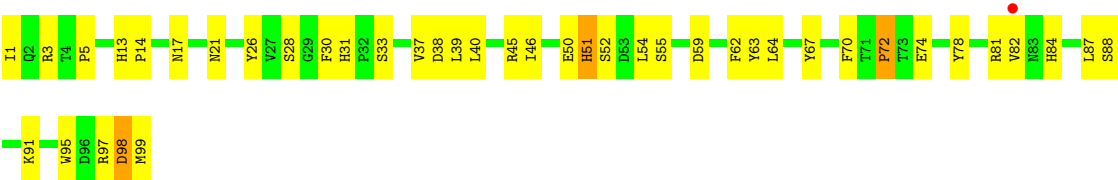
- Molecule 2: Beta-2-microglobulin

Chain F:



- Molecule 2: Beta-2-microglobulin

Chain H:



● Molecule 3: DIMERIC PEPTIDE INHIBITOR

Chain I:



● Molecule 3: DIMERIC PEPTIDE INHIBITOR

Chain J:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.05Å 158.43Å 82.54Å 90.00° 90.11° 90.00°	Depositor
Resolution (Å)	37.24 – 3.10 37.22 – 3.08	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.24-3.10) 89.5 (37.22-3.08)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 3.06Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.314 , 0.397 0.293 , 0.334	Depositor DCC
R_{free} test set	1475 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	96.3	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 37.3	EDS
Estimated twinning fraction	0.390 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 29025 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11241	wwPDB-VP
Average B, all atoms (Å ²)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LE1, MLE, SAR

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	0.41	0/2020	0.57	0/2764
1	C	0.40	0/2020	0.58	0/2764
1	E	0.42	0/2020	0.60	1/2764 (0.0%)
1	G	0.39	0/2020	0.55	0/2764
2	B	0.38	0/831	0.56	0/1130
2	D	0.41	0/831	0.57	0/1130
2	F	0.39	0/831	0.57	0/1130
2	H	0.45	0/831	0.60	0/1130
3	I	0.48	0/63	0.43	0/83
3	J	0.50	0/74	0.39	0/96
All	All	0.41	0/11541	0.57	1/15755 (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
3	I	0	3
3	J	0	2
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	30	LEU	CA-CB-CG	5.54	128.04	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	I	3	LE1	Mainchain,Peptide
3	I	8	GLY	Peptide
3	J	102	PHE	Mainchain
3	J	103	LE1	Mainchain

5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1958	0	1753	79	0
1	C	1958	0	1753	80	0
1	E	1958	0	1753	72	0
1	G	1958	0	1753	73	0
2	B	808	0	741	27	0
2	D	808	0	741	25	0
2	F	808	0	741	25	0
2	H	808	0	741	23	0
3	I	83	0	75	3	0
3	J	94	0	82	2	0
All	All	11241	0	10133	395	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 18.

All (395) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:84:GLY:HA3	1:G:88:TYR:OH	1.53	1.07
1:C:150:LYS:O	1:C:154:PHE:HB2	1.57	1.03
2:H:84:HIS:H	2:H:87:LEU:HD12	1.33	0.91
1:A:6:SER:CB	1:A:97:GLU:HB3	2.00	0.91
2:H:17:ASN:ND2	2:H:74:GLU:OE1	2.05	0.90
1:A:6:SER:HB3	1:A:97:GLU:HB3	1.54	0.86
1:A:22:PRO:HB3	1:A:39:ASN:HB2	1.60	0.81
1:G:146:LYS:O	1:G:150:LYS:HG3	1.81	0.80
1:A:252:CYS:HB3	1:A:265:VAL:HB	1.63	0.80
2:D:26:TYR:HB2	2:D:65:LEU:HD13	1.64	0.80

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:159:CYS:HB3	1:A:160:PRO:HD3	1.64	0.80
1:A:84:GLY:HA3	1:A:88:TYR:OH	1.82	0.79
1:E:6:SER:HB3	1:E:97:GLU:HB3	1.64	0.78
1:A:67:ASP:OD2	1:A:162:ARG:NH2	2.15	0.78
1:C:247:GLU:CD	1:C:247:GLU:H	1.86	0.78
2:F:96:ASP:HB3	2:F:99:MET:HB2	1.66	0.78
1:A:12:THR:HG23	1:A:91:GLN:HG2	1.66	0.77
2:D:40:LEU:HB3	2:D:43:GLY:HA2	1.65	0.77
1:E:94:LEU:HD12	1:E:108:ALA:HA	1.66	0.77
1:C:94:LEU:HA	1:C:107:THR:O	1.85	0.76
1:G:213:LEU:O	1:G:250:TYR:HA	1.86	0.75
1:C:24:PHE:HB3	1:C:40:SER:HB3	1.66	0.75
1:A:38:TYR:OH	1:A:69:ARG:HG3	1.86	0.74
1:C:159:CYS:HB3	1:C:160:PRO:HD3	1.68	0.74
2:F:2:GLN:HG2	2:F:32:PRO:HD3	1.69	0.74
2:F:49:VAL:HG12	2:F:66:TYR:HD2	1.52	0.74
1:E:261:GLN:HG3	1:E:262:PRO:HD2	1.70	0.73
2:D:81:ARG:HD3	2:D:90:PRO:HB2	1.69	0.73
1:G:42:ARG:HH21	1:G:44:GLU:HB3	1.54	0.70
1:E:6:SER:CB	1:E:97:GLU:HB3	2.21	0.70
1:C:35:TYR:O	1:C:47:PRO:HA	1.92	0.69
1:C:22:PRO:HA	1:C:41:LEU:HD13	1.74	0.69
2:B:7:ILE:HG23	2:B:27:VAL:HG22	1.75	0.68
1:G:133:GLU:HA	1:G:136:ALA:HB3	1.74	0.68
1:A:167:LEU:O	1:A:171:ARG:HB2	1.94	0.68
2:B:13:HIS:HB2	2:B:21:ASN:HD21	1.59	0.67
1:A:77:GLU:HG3	1:A:140:ARG:HE	1.58	0.67
1:A:196:LEU:O	1:A:239:SER:HA	1.95	0.66
1:G:71:LYS:HA	1:G:74:LEU:HD12	1.77	0.66
2:D:54:LEU:HD12	2:D:64:LEU:HD12	1.78	0.65
1:G:110:PHE:HB2	1:G:118:MET:HB2	1.77	0.65
1:E:205:PRO:O	1:E:256:HIS:CE1	2.50	0.64
2:D:30:PHE:CE2	2:D:62:PHE:HB2	2.33	0.64
1:C:203:PHE:HB2	1:C:256:HIS:CE1	2.33	0.64
1:A:261:GLN:HG3	1:A:262:PRO:HD2	1.79	0.64
1:A:45:ALA:H	1:A:65:THR:HG23	1.63	0.64
1:E:253:ILE:HD13	1:E:264:ARG:HA	1.78	0.64
1:E:159:CYS:HB3	1:E:160:PRO:HD3	1.78	0.64
1:C:22:PRO:HB3	1:C:39:ASN:HB2	1.79	0.64
1:C:57:VAL:O	1:C:59:TRP:N	2.30	0.63
1:C:160:PRO:HA	1:C:163:LEU:HB3	1.81	0.63
2:F:2:GLN:NE2	2:F:86:THR:HG23	2.14	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:162:ARG:O	1:E:166:HIS:CD2	2.52	0.63
1:G:98:LEU:HG	1:G:163:LEU:HD23	1.80	0.62
1:G:57:VAL:O	1:G:59:TRP:N	2.32	0.62
2:H:78:TYR:HB2	2:H:95:TRP:HE3	1.64	0.62
1:A:149:ASN:C	1:A:151:GLU:H	2.03	0.61
1:E:196:LEU:O	1:E:239:SER:HA	2.01	0.61
1:C:110:PHE:HB2	1:C:118:MET:HB2	1.81	0.61
1:G:256:HIS:HD2	1:G:258:GLY:H	1.49	0.61
1:C:22:PRO:CB	1:C:39:ASN:HB2	2.30	0.60
1:G:91:GLN:HB2	1:G:111:ALA:HB3	1.82	0.60
1:G:122:LEU:HD12	1:G:122:LEU:H	1.65	0.60
1:E:77:GLU:HG3	1:E:140:ARG:HE	1.66	0.60
1:G:65:THR:HA	1:G:68:LEU:HD12	1.84	0.60
1:A:247:GLU:O	1:A:250:TYR:HB2	2.01	0.60
1:A:256:HIS:CD2	1:A:258:GLY:H	2.20	0.60
2:F:23:LEU:HB2	2:F:70:PHE:CE1	2.37	0.60
1:C:11:LEU:HD21	1:C:71:LYS:HG2	1.84	0.60
1:G:101:ASP:HB2	1:G:103:THR:OG1	2.02	0.60
1:E:196:LEU:HD12	1:E:242:VAL:HG11	1.84	0.59
2:F:27:VAL:HG21	2:F:82:VAL:HG21	1.83	0.59
1:A:213:LEU:CD2	1:A:218:ALA:HA	2.33	0.59
1:C:157:PHE:O	1:C:160:PRO:HD2	2.02	0.59
1:C:25:TRP:HZ2	2:D:54:LEU:HD22	1.66	0.59
1:A:222:GLY:HA3	1:A:239:SER:O	2.02	0.59
1:G:144:GLN:HA	1:G:144:GLN:OE1	2.01	0.59
1:E:104:SER:O	1:E:106:PRO:HD3	2.03	0.59
2:F:81:ARG:HD3	2:F:90:PRO:HB2	1.84	0.59
1:A:11:LEU:HG	1:A:26:VAL:HG13	1.85	0.59
1:C:183:ARG:HG2	2:D:98:ASP:OD1	2.02	0.59
1:G:84:GLY:HA3	1:G:88:TYR:HH	1.65	0.58
1:C:178:GLU:O	1:C:203:PHE:HA	2.02	0.58
2:B:56:PHE:HA	2:B:62:PHE:HA	1.85	0.58
1:C:189:SER:H	1:C:194:SER:HA	1.68	0.58
1:C:24:PHE:O	1:C:40:SER:N	2.36	0.57
1:E:22:PRO:HB2	1:E:24:PHE:O	2.03	0.57
1:G:244:SER:HA	1:G:247:GLU:OE1	2.04	0.57
1:A:222:GLY:HA2	1:A:240:LEU:HD13	1.86	0.57
1:A:184:LEU:HD22	1:A:252:CYS:HB2	1.86	0.57
1:E:148:ALA:O	1:E:151:GLU:HB2	2.05	0.57
2:H:50:GLU:HB3	2:H:67:TYR:CZ	2.40	0.57
1:E:59:TRP:HA	1:E:62:GLU:OE1	2.05	0.57
1:A:56:GLN:C	1:A:169:ARG:HH21	2.07	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:25:TRP:CZ2	2:D:54:LEU:HD22	2.38	0.56
1:G:7:LEU:HD21	1:G:9:TYR:HE1	1.70	0.56
2:B:5:PRO:HB3	2:B:30:PHE:HB3	1.88	0.56
1:C:68:LEU:O	1:C:71:LYS:N	2.38	0.56
1:G:159:CYS:HB3	1:G:160:PRO:HD3	1.88	0.56
1:A:205:PRO:O	1:A:256:HIS:HE1	1.89	0.56
1:G:160:PRO:HA	1:G:163:LEU:HB3	1.88	0.56
1:C:196:LEU:HD12	1:C:242:VAL:HG11	1.87	0.56
1:C:98:LEU:HG	1:C:163:LEU:HD21	1.86	0.56
1:E:117:PHE:HD2	1:E:134:ALA:HB2	1.71	0.56
2:B:5:PRO:HB2	2:B:27:VAL:HG12	1.88	0.56
2:B:27:VAL:HG21	2:B:82:VAL:HG21	1.87	0.55
1:G:30:LEU:CD2	1:G:35:TYR:HB3	2.37	0.55
1:C:154:PHE:O	1:C:159:CYS:HB2	2.06	0.55
1:G:25:TRP:HB2	1:G:38:TYR:O	2.06	0.55
2:F:42:ASN:HD21	2:F:76:ASP:HA	1.71	0.55
1:G:24:PHE:HB3	1:G:40:SER:HB3	1.87	0.55
1:C:131:TRP:HB3	1:C:132:PRO:CD	2.37	0.55
2:D:54:LEU:HD21	2:D:62:PHE:CD1	2.42	0.55
2:F:5:PRO:HA	2:F:30:PHE:HB3	1.88	0.54
1:A:71:LYS:HA	1:A:74:LEU:HD12	1.89	0.54
1:A:94:LEU:HD12	1:A:108:ALA:HA	1.89	0.54
2:H:5:PRO:HG3	2:H:84:HIS:HB2	1.89	0.54
1:G:256:HIS:CD2	1:G:258:GLY:H	2.23	0.54
2:H:40:LEU:HD23	2:H:45:ARG:HA	1.90	0.54
1:C:194:SER:O	1:C:242:VAL:HG22	2.08	0.54
1:E:138:SER:O	1:E:142:GLN:HG2	2.08	0.54
2:H:30:PHE:HE2	2:H:33:SER:HA	1.73	0.54
1:A:127:TRP:CZ3	1:A:141:TRP:HB3	2.43	0.54
1:E:162:ARG:O	1:E:166:HIS:HD2	1.90	0.54
2:F:9:VAL:HG11	2:F:95:TRP:HB2	1.89	0.54
1:E:55:ASN:O	1:E:169:ARG:NE	2.38	0.54
1:A:43:GLY:O	1:A:69:ARG:NH2	2.30	0.54
1:E:106:PRO:HB3	1:E:155:LEU:HD22	1.88	0.53
1:E:155:LEU:O	1:E:160:PRO:HD3	2.08	0.53
1:E:205:PRO:HB2	1:E:207:GLU:OE2	2.07	0.53
1:G:200:ALA:HB3	1:G:236:ALA:HB3	1.89	0.53
2:B:13:HIS:HB2	2:B:21:ASN:ND2	2.22	0.53
1:E:180:PRO:HB3	1:E:203:PHE:HB3	1.89	0.53
2:H:26:TYR:OH	2:H:28:SER:HB3	2.09	0.53
1:G:117:PHE:HD2	1:G:134:ALA:HB2	1.74	0.53
1:C:180:PRO:HB3	1:C:203:PHE:HD1	1.74	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:108:ALA:O	1:G:109:LYS:HG3	2.08	0.53
2:H:51:HIS:O	2:H:51:HIS:CG	2.61	0.53
1:A:205:PRO:HB2	1:A:206:PRO:HD2	1.91	0.53
1:G:22:PRO:HA	1:G:41:LEU:HD13	1.90	0.53
1:C:36:LEU:HD23	1:C:36:LEU:C	2.29	0.53
1:C:184:LEU:HB3	1:C:267:LEU:HA	1.91	0.53
1:A:6:SER:HB2	1:A:97:GLU:HB3	1.89	0.52
1:A:80:LYS:HB3	1:A:140:ARG:NH2	2.24	0.52
1:E:222:GLY:HA2	1:E:240:LEU:HD13	1.91	0.52
2:B:40:LEU:HD12	2:B:79:ALA:HB3	1.91	0.52
1:G:81:ALA:HB2	1:G:140:ARG:HD2	1.91	0.52
1:G:162:ARG:O	1:G:166:HIS:HD2	1.93	0.52
1:E:58:SER:C	1:E:60:TYR:H	2.13	0.52
2:H:81:ARG:HA	2:H:91:LYS:O	2.09	0.52
1:E:93:LEU:HD13	2:F:56:PHE:CE1	2.45	0.52
1:A:161:HIS:ND1	1:A:165:GLU:OE2	2.43	0.52
1:C:6:SER:O	1:C:31:GLY:N	2.42	0.52
1:A:210:LEU:O	1:A:221:THR:HG22	2.10	0.52
2:D:6:LYS:HB3	2:D:28:SER:O	2.10	0.51
1:A:39:ASN:O	1:A:43:GLY:HA2	2.11	0.51
1:C:180:PRO:HB3	1:C:203:PHE:CD1	2.46	0.51
2:B:31:HIS:HA	2:B:32:PRO:O	2.10	0.51
1:E:178:GLU:N	1:E:204:TYR:O	2.43	0.51
1:A:253:ILE:CD1	1:A:264:ARG:HG2	2.41	0.51
1:E:64:GLU:OE1	1:E:162:ARG:HD3	2.11	0.51
1:C:7:LEU:HD23	1:C:163:LEU:HB2	1.93	0.50
1:C:229:ASN:HD22	1:C:229:ASN:N	2.09	0.50
2:H:17:ASN:HA	2:H:72:PRO:HB2	1.92	0.50
2:F:5:PRO:HD3	2:F:86:THR:OG1	2.11	0.50
2:H:1:ILE:HD13	2:H:3:ARG:HG3	1.93	0.50
1:G:13:ALA:HA	1:G:23:ALA:O	2.11	0.50
1:C:42:ARG:HH21	1:C:44:GLU:HB3	1.77	0.50
1:E:6:SER:CA	1:E:97:GLU:HB3	2.41	0.50
2:F:2:GLN:HE21	2:F:86:THR:HG23	1.76	0.50
1:C:22:PRO:HD3	1:C:41:LEU:HD22	1.92	0.50
1:G:47:PRO:HG2	1:G:52:VAL:HG13	1.94	0.50
2:F:51:HIS:HB3	2:F:66:TYR:CZ	2.47	0.50
1:A:93:LEU:HB3	1:A:109:LYS:HB2	1.94	0.50
1:G:205:PRO:HB2	1:G:206:PRO:HD2	1.94	0.50
1:A:231:ASP:H	2:B:12:ARG:HH21	1.60	0.50
2:D:51:HIS:CG	2:D:51:HIS:O	2.64	0.50
2:H:97:ARG:O	2:H:98:ASP:HB2	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:229:ASN:HD21	1:G:235:HIS:HB2	1.76	0.50
1:E:39:ASN:O	1:E:43:GLY:N	2.42	0.50
1:G:22:PRO:CB	1:G:39:ASN:HB2	2.42	0.50
1:A:69:ARG:O	1:A:72:GLU:HB3	2.11	0.50
2:F:96:ASP:C	2:F:98:ASP:H	2.15	0.49
1:E:205:PRO:O	1:E:256:HIS:HE1	1.94	0.49
1:C:56:GLN:HA	1:C:56:GLN:OE1	2.12	0.49
1:E:67:ASP:HB3	1:E:154:PHE:HE2	1.76	0.49
1:E:197:THR:HG21	2:F:99:MET:HA	1.95	0.49
2:B:5:PRO:HB2	2:B:27:VAL:CG1	2.43	0.49
1:C:96:CYS:HA	1:C:106:PRO:HA	1.95	0.49
2:D:55:SER:O	2:D:62:PHE:HA	2.13	0.48
1:C:26:VAL:HG12	1:C:27:SER:N	2.28	0.48
2:D:17:ASN:HD21	2:D:74:GLU:HB2	1.78	0.48
1:E:97:GLU:O	1:E:104:SER:HA	2.12	0.48
2:F:5:PRO:CA	2:F:30:PHE:HB3	2.43	0.48
2:B:83:ASN:HA	2:B:87:LEU:HD12	1.94	0.48
1:A:171:ARG:HD2	1:A:175:GLU:HB2	1.96	0.48
1:A:127:TRP:CD2	1:A:141:TRP:HE3	2.31	0.48
2:D:26:TYR:CZ	2:D:28:SER:HB3	2.49	0.48
2:D:42:ASN:HD21	2:D:76:ASP:HA	1.79	0.48
1:E:57:VAL:O	1:E:59:TRP:CD1	2.67	0.48
2:D:40:LEU:HB3	2:D:43:GLY:CA	2.40	0.48
1:G:59:TRP:HA	1:G:62:GLU:OE1	2.14	0.48
1:A:47:PRO:HB3	1:A:61:TRP:CZ2	2.49	0.48
2:F:40:LEU:O	2:F:78:TYR:HA	2.13	0.48
1:G:22:PRO:HB3	1:G:39:ASN:HB2	1.95	0.48
3:I:9:SAR:HA3	3:I:10:MLE:HN1	1.57	0.48
1:A:30:LEU:HD22	1:A:35:TYR:CE1	2.49	0.48
1:G:71:LYS:O	1:G:74:LEU:HB2	2.14	0.47
1:E:222:GLY:HA2	1:E:240:LEU:CD1	2.44	0.47
1:E:160:PRO:O	1:E:164:ARG:N	2.43	0.47
1:C:203:PHE:HE2	1:C:206:PRO:HA	1.79	0.47
1:A:26:VAL:HG12	1:A:27:SER:N	2.29	0.47
1:C:14:VAL:HG12	1:C:89:THR:HG23	1.95	0.47
1:G:74:LEU:O	1:G:77:GLU:HB3	2.14	0.47
1:C:98:LEU:HG	1:C:163:LEU:CD2	2.44	0.47
2:H:38:ASP:OD2	2:H:81:ARG:NH1	2.47	0.47
1:A:230:SER:OG	2:B:12:ARG:NH2	2.47	0.47
1:A:82:LEU:HA	3:I:11:TYR:OH	2.14	0.47
2:H:78:TYR:CB	2:H:95:TRP:HE3	2.28	0.47
1:A:26:VAL:HG21	1:A:68:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:22:PRO:HD3	1:E:41:LEU:HD22	1.95	0.47
2:D:39:LEU:HB3	2:D:46:ILE:HD12	1.96	0.47
1:C:33:GLN:OE1	1:C:51:TRP:HZ2	1.97	0.47
1:G:38:TYR:OH	1:G:69:ARG:HG3	2.14	0.47
2:F:59:ASP:O	2:F:60:TRP:HB2	2.14	0.46
3:J:102:PHE:HA	3:J:112:PRO:HA	1.97	0.46
1:E:101:ASP:C	1:E:103:THR:H	2.19	0.46
1:E:94:LEU:HA	1:E:107:THR:O	2.16	0.46
1:A:253:ILE:HD13	1:A:264:ARG:HA	1.96	0.46
2:H:54:LEU:HD21	2:H:62:PHE:CD1	2.49	0.46
1:A:174:LEU:O	1:A:176:TRP:N	2.48	0.46
1:E:203:PHE:CE2	1:E:234:PHE:HB3	2.51	0.46
1:G:229:ASN:H	1:G:229:ASN:HD22	1.63	0.46
2:B:49:VAL:HG22	2:B:68:THR:HB	1.97	0.46
1:E:38:TYR:CD2	1:E:38:TYR:C	2.89	0.46
1:A:62:GLU:HA	1:A:65:THR:OG1	2.15	0.46
2:H:26:TYR:CE1	2:H:63:TYR:HB2	2.51	0.46
1:C:179:PRO:HA	1:C:256:HIS:CD2	2.51	0.46
1:A:56:GLN:HG2	1:A:61:TRP:NE1	2.31	0.46
1:E:117:PHE:CD2	1:E:134:ALA:HB2	2.51	0.46
1:E:115:GLU:O	1:E:116:GLU:C	2.54	0.46
1:C:210:LEU:O	1:C:221:THR:HG23	2.16	0.46
1:A:159:CYS:HB3	1:A:160:PRO:CD	2.42	0.46
1:C:180:PRO:HA	1:C:202:SER:O	2.15	0.45
2:F:83:ASN:HB2	2:F:90:PRO:HB3	1.98	0.45
1:C:186:ALA:HB2	1:C:196:LEU:HD21	1.99	0.45
1:G:162:ARG:O	1:G:166:HIS:CD2	2.69	0.45
1:E:174:LEU:O	1:E:176:TRP:N	2.49	0.45
1:G:60:TYR:C	1:G:62:GLU:H	2.19	0.45
1:E:59:TRP:O	1:E:63:LYS:HB2	2.16	0.45
1:G:188:PRO:HA	1:G:194:SER:HA	1.99	0.45
1:G:228:PRO:HA	1:G:234:PHE:HA	1.97	0.45
1:C:112:LEU:O	1:C:113:ASN:C	2.55	0.45
1:G:229:ASN:HD22	1:G:229:ASN:N	2.15	0.45
1:E:46:GLU:HA	1:E:47:PRO:HD2	1.69	0.45
1:C:13:ALA:HB2	1:C:24:PHE:HD1	1.80	0.45
1:A:81:ALA:HB2	1:A:140:ARG:HD2	1.98	0.45
1:E:15:SER:HG	1:E:88:TYR:H	1.62	0.45
1:C:159:CYS:HB3	1:C:160:PRO:CD	2.44	0.45
1:C:203:PHE:HB2	1:C:256:HIS:NE2	2.32	0.45
2:F:56:PHE:C	2:F:63:TYR:HE2	2.21	0.45
1:E:174:LEU:HD22	1:E:174:LEU:H	1.81	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:200:ALA:O	1:A:235:HIS:ND1	2.50	0.44
1:E:200:ALA:HB3	1:E:236:ALA:HB3	1.98	0.44
1:E:17:PRO:HG3	1:E:23:ALA:HB2	2.00	0.44
1:A:98:LEU:HG	1:A:163:LEU:HD23	1.99	0.44
1:G:66:THR:HA	1:G:69:ARG:HD2	1.99	0.44
1:A:42:ARG:NH2	1:A:44:GLU:HB3	2.32	0.44
1:A:36:LEU:C	1:A:36:LEU:HD23	2.38	0.44
1:C:65:THR:HG22	1:C:69:ARG:NE	2.32	0.44
1:G:18:ALA:O	1:G:21:THR:HB	2.17	0.44
1:E:64:GLU:OE1	1:E:162:ARG:NH1	2.49	0.44
1:G:6:SER:O	1:G:31:GLY:N	2.51	0.44
2:H:31:HIS:HD2	2:H:62:PHE:CE2	2.36	0.44
2:B:26:TYR:CE1	2:B:63:TYR:HB2	2.52	0.44
2:B:32:PRO:HB2	2:B:33:SER:H	1.63	0.44
1:A:253:ILE:HA	1:A:263:LEU:O	2.17	0.44
1:A:201:PHE:CD1	2:B:14:PRO:HG3	2.52	0.44
1:C:7:LEU:HD11	1:C:9:TYR:CE1	2.51	0.44
1:C:244:SER:HA	1:C:247:GLU:OE1	2.17	0.44
1:E:178:GLU:HA	1:E:179:PRO:HD3	1.90	0.44
2:D:83:ASN:HA	2:D:87:LEU:HD12	1.99	0.44
1:C:253:ILE:HD12	1:C:264:ARG:HG2	2.00	0.44
1:G:10:HIS:O	1:G:26:VAL:HA	2.18	0.44
1:A:13:ALA:HB2	1:A:24:PHE:HD1	1.83	0.44
1:E:242:VAL:HB	1:E:250:TYR:CE1	2.53	0.43
1:C:193:PHE:HA	1:C:242:VAL:O	2.18	0.43
1:G:67:ASP:OD2	1:G:162:ARG:NH2	2.51	0.43
1:G:50:ALA:O	1:G:52:VAL:N	2.51	0.43
1:C:228:PRO:HA	1:C:234:PHE:HA	1.99	0.43
1:E:109:LYS:HD3	1:E:109:LYS:HA	1.74	0.43
2:H:21:ASN:N	2:H:70:PHE:O	2.50	0.43
1:G:178:GLU:HA	1:G:179:PRO:HD2	1.87	0.43
1:G:132:PRO:O	1:G:136:ALA:N	2.51	0.43
1:A:54:GLU:O	1:A:56:GLN:N	2.51	0.43
1:A:29:TRP:HA	1:A:33:GLN:O	2.18	0.43
1:E:243:LYS:O	1:E:246:ASP:HB3	2.18	0.43
2:B:70:PHE:CE2	2:B:72:PRO:HB3	2.54	0.43
2:B:58:LYS:C	2:B:60:TRP:H	2.21	0.43
1:C:17:PRO:HG3	1:C:23:ALA:HB2	2.00	0.43
1:A:112:LEU:HB2	1:A:117:PHE:CZ	2.53	0.43
1:A:93:LEU:HD13	2:B:56:PHE:HE1	1.84	0.43
1:C:224:GLY:O	1:C:225:ASP:HB2	2.18	0.43
1:G:98:LEU:HG	1:G:163:LEU:CD2	2.48	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:31:HIS:O	2:B:84:HIS:HE1	2.01	0.43
1:A:89:THR:O	1:A:112:LEU:HD12	2.18	0.43
1:E:214:ARG:O	1:E:215:ASN:C	2.57	0.43
1:E:8:LEU:HD23	1:E:95:GLY:HA3	2.00	0.43
1:G:210:LEU:HD22	1:G:252:CYS:SG	2.59	0.43
1:E:223:GLN:O	1:E:238:SER:HA	2.19	0.43
1:G:117:PHE:CD2	1:G:134:ALA:HB2	2.54	0.43
2:D:84:HIS:H	2:D:87:LEU:HD12	1.84	0.43
1:C:169:ARG:H	1:C:169:ARG:HG3	1.66	0.43
1:G:133:GLU:HA	1:G:136:ALA:CB	2.46	0.42
1:E:256:HIS:CD2	1:E:258:GLY:H	2.36	0.42
2:D:17:ASN:ND2	2:D:74:GLU:HB2	2.34	0.42
1:A:214:ARG:O	1:A:215:ASN:C	2.57	0.42
1:C:247:GLU:CD	1:C:247:GLU:N	2.62	0.42
1:E:77:GLU:HG3	1:E:140:ARG:HH21	1.83	0.42
1:C:186:ALA:HB2	1:C:196:LEU:CD2	2.49	0.42
2:F:56:PHE:C	2:F:63:TYR:CE2	2.93	0.42
1:A:165:GLU:O	1:A:168:GLU:N	2.52	0.42
1:C:167:LEU:O	1:C:167:LEU:HG	2.20	0.42
1:A:201:PHE:HB3	2:B:12:ARG:O	2.19	0.42
1:G:203:PHE:HB2	1:G:256:HIS:CE1	2.54	0.42
1:A:206:PRO:O	1:A:208:LEU:N	2.52	0.42
2:H:13:HIS:HB3	2:H:14:PRO:HD2	2.01	0.42
1:G:59:TRP:O	1:G:63:LYS:HB2	2.20	0.42
1:A:47:PRO:HG3	1:A:61:TRP:CE2	2.54	0.42
2:B:31:HIS:ND1	2:B:32:PRO:HA	2.35	0.42
1:C:174:LEU:C	1:C:176:TRP:H	2.23	0.42
1:E:231:ASP:OD1	1:E:233:SER:OG	2.34	0.42
1:G:155:LEU:O	1:G:159:CYS:HB3	2.19	0.42
1:A:159:CYS:CB	1:A:160:PRO:HD3	2.43	0.42
2:F:27:VAL:CG2	2:F:82:VAL:HG21	2.50	0.42
1:C:42:ARG:C	1:C:44:GLU:H	2.22	0.42
2:B:9:VAL:HG11	2:B:95:TRP:HB2	2.02	0.42
1:E:53:TRP:CE3	1:E:53:TRP:HA	2.54	0.42
1:C:68:LEU:O	1:C:71:LYS:HB2	2.20	0.42
1:C:56:GLN:HE21	1:C:166:HIS:CE1	2.38	0.42
1:A:22:PRO:HA	1:A:41:LEU:HD13	2.02	0.41
1:C:11:LEU:HD11	1:C:94:LEU:HD22	2.01	0.41
1:C:66:THR:O	1:C:70:ILE:HG13	2.20	0.41
1:A:65:THR:H	1:A:65:THR:HG1	1.53	0.41
1:G:180:PRO:HB3	1:G:203:PHE:HB3	2.03	0.41
1:G:154:PHE:HA	1:G:158:SER:OG	2.20	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:38:TYR:OH	1:G:69:ARG:CG	2.69	0.41
1:A:8:LEU:HD23	1:A:94:LEU:O	2.21	0.41
2:B:84:HIS:HB3	2:B:87:LEU:HG	2.02	0.41
1:C:33:GLN:OE1	1:C:51:TRP:CZ2	2.73	0.41
1:C:152:LEU:O	1:C:156:LEU:HB2	2.20	0.41
1:C:135:LEU:HA	1:C:135:LEU:HD23	1.90	0.41
3:I:5:GLY:C	3:I:7:PHE:N	2.73	0.41
2:D:44:GLU:O	2:D:45:ARG:C	2.59	0.41
1:A:171:ARG:HA	1:A:174:LEU:HD23	2.02	0.41
1:C:110:PHE:CD1	1:C:110:PHE:N	2.88	0.41
2:H:39:LEU:HB3	2:H:46:ILE:HD12	2.02	0.41
1:C:38:TYR:C	1:C:38:TYR:CD2	2.94	0.41
1:E:213:LEU:HD23	1:E:218:ALA:HA	2.03	0.41
1:E:161:HIS:ND1	1:E:165:GLU:OE2	2.53	0.41
1:G:96:CYS:SG	1:G:160:PRO:HD3	2.61	0.41
1:E:93:LEU:HD13	2:F:56:PHE:HE1	1.85	0.41
1:A:118:MET:HA	1:A:128:GLY:O	2.21	0.41
1:E:173:ASN:O	1:E:176:TRP:HB3	2.21	0.41
1:G:54:GLU:OE1	1:G:56:GLN:NE2	2.54	0.41
2:D:21:ASN:CG	2:D:22:PHE:H	2.24	0.41
1:A:138:SER:O	1:A:142:GLN:HG2	2.21	0.41
1:G:252:CYS:HB3	1:G:265:VAL:HB	2.03	0.41
2:H:37:VAL:HG13	2:H:82:VAL:HG22	2.02	0.41
1:E:78:ALA:C	1:E:80:LYS:H	2.24	0.41
1:C:18:ALA:O	1:C:21:THR:HB	2.20	0.41
2:F:17:ASN:HA	2:F:72:PRO:O	2.21	0.41
1:G:72:GLU:C	1:G:74:LEU:N	2.75	0.41
2:D:97:ARG:O	2:D:98:ASP:HB2	2.21	0.41
1:E:6:SER:HA	1:E:97:GLU:HB3	2.03	0.40
1:E:36:LEU:HD12	1:E:61:TRP:HZ3	1.86	0.40
2:H:59:ASP:OD1	2:H:59:ASP:C	2.60	0.40
1:C:91:GLN:NE2	2:D:60:TRP:HB3	2.36	0.40
1:A:205:PRO:CB	1:A:206:PRO:HD2	2.51	0.40
1:E:235:HIS:CG	1:E:236:ALA:N	2.89	0.40
1:C:204:TYR:CD2	1:C:205:PRO:HA	2.56	0.40
1:G:203:PHE:HD2	1:G:256:HIS:HE1	1.69	0.40
2:B:50:GLU:HB3	2:B:67:TYR:CZ	2.57	0.40
1:A:174:LEU:C	1:A:176:TRP:N	2.75	0.40
1:A:149:ASN:C	1:A:151:GLU:N	2.72	0.40
1:G:56:GLN:OE1	1:G:56:GLN:HA	2.21	0.40
2:B:10:TYR:CE2	2:B:24:ASN:HB2	2.57	0.40
1:C:122:LEU:HD12	1:C:122:LEU:H	1.86	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:186:ALA:HA	1:E:195:VAL:O	2.22	0.40
3:J:109:SAR:HA3	3:J:110:MLE:HN1	1.78	0.40
1:G:77:GLU:OE2	1:G:140:ARG:NH2	2.54	0.40
1:G:50:ALA:C	1:G:52:VAL:H	2.25	0.40
1:C:116:GLU:HB2	2:D:60:TRP:HE1	1.86	0.40
1:C:214:ARG:HA	1:C:250:TYR:HA	2.03	0.40
1:G:173:ASN:O	1:G:176:TRP:HB3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	261/267 (98%)	215 (82%)	39 (15%)	7 (3%)	8	39
1	C	261/267 (98%)	213 (82%)	38 (15%)	10 (4%)	5	30
1	E	261/267 (98%)	219 (84%)	33 (13%)	9 (3%)	6	32
1	G	261/267 (98%)	224 (86%)	30 (12%)	7 (3%)	8	39
2	B	97/99 (98%)	84 (87%)	12 (12%)	1 (1%)	22	68
2	D	97/99 (98%)	82 (84%)	14 (14%)	1 (1%)	22	68
2	F	97/99 (98%)	84 (87%)	12 (12%)	1 (1%)	22	68
2	H	97/99 (98%)	81 (84%)	14 (14%)	2 (2%)	11	48
3	I	7/16 (44%)	6 (86%)	1 (14%)	0	100	100
3	J	7/16 (44%)	5 (71%)	2 (29%)	0	100	100
All	All	1446/1496 (97%)	1213 (84%)	195 (14%)	38 (3%)	8	41

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	C	58	SER
1	C	215	ASN

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Mol	Chain	Res	Type
1	G	58	SER
1	G	202	SER
1	A	100	PRO
1	A	207	GLU
1	C	202	SER
1	C	225	ASP
1	E	59	TRP
1	E	100	PRO
1	E	166	HIS
1	E	175	GLU
1	E	193	PHE
1	G	189	SER
2	H	98	ASP
1	A	175	GLU
1	A	191	PRO
1	C	65	THR
1	C	113	ASN
2	D	45	ARG
1	E	58	SER
1	E	215	ASN
1	G	51	TRP
1	G	113	ASN
1	A	58	SER
1	A	215	ASN
1	C	38	TYR
1	C	57	VAL
1	C	219	ALA
1	E	116	GLU
2	F	14	PRO
2	B	32	PRO
1	C	262	PRO
1	G	57	VAL
1	G	262	PRO
1	E	180	PRO
2	H	72	PRO

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	186/220 (84%)	163 (88%)	23 (12%)	7	25
1	C	186/220 (84%)	163 (88%)	23 (12%)	7	25
1	E	186/220 (84%)	165 (89%)	21 (11%)	9	32
1	G	186/220 (84%)	168 (90%)	18 (10%)	12	41
2	B	88/94 (94%)	78 (89%)	10 (11%)	8	31
2	D	88/94 (94%)	83 (94%)	5 (6%)	29	70
2	F	88/94 (94%)	77 (88%)	11 (12%)	7	25
2	H	88/94 (94%)	82 (93%)	6 (7%)	22	62
3	I	6/9 (67%)	5 (83%)	1 (17%)	3	11
3	J	7/9 (78%)	7 (100%)	0	100	100
All	All	1109/1274 (87%)	991 (89%)	118 (11%)	10	35

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	27	SER
1	A	30	LEU
1	A	41	LEU
1	A	62	GLU
1	A	65	THR
1	A	71	LYS
1	A	80	LYS
1	A	94	LEU
1	A	105	VAL
1	A	117	PHE
1	A	133	GLU
1	A	140	ARG
1	A	155	LEU
1	A	183	ARG
1	A	198	CYS
1	A	202	SER
1	A	225	ASP
1	A	226	PHE
1	A	247	GLU
1	A	251	CYS
1	A	259	LEU
1	A	261	GLN
2	B	2	GLN

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Mol	Chain	Res	Type
2	B	28	SER
2	B	34	ASP
2	B	35	ILE
2	B	42	ASN
2	B	50	GLU
2	B	54	LEU
2	B	64	LEU
2	B	70	PHE
2	B	81	ARG
1	C	7	LEU
1	C	21	THR
1	C	33	GLN
1	C	41	LEU
1	C	66	THR
1	C	67	ASP
1	C	80	LYS
1	C	82	LEU
1	C	94	LEU
1	C	98	LEU
1	C	103	THR
1	C	126	THR
1	C	130	ASP
1	C	168	GLU
1	C	174	LEU
1	C	181	SER
1	C	183	ARG
1	C	195	VAL
1	C	221	THR
1	C	229	ASN
1	C	230	SER
1	C	241	THR
1	C	251	CYS
2	D	33	SER
2	D	55	SER
2	D	61	SER
2	D	64	LEU
2	D	92	ILE
1	E	21	THR
1	E	26	VAL
1	E	36	LEU
1	E	38	TYR
1	E	65	THR

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Mol	Chain	Res	Type
1	E	80	LYS
1	E	82	LEU
1	E	94	LEU
1	E	103	THR
1	E	105	VAL
1	E	124	GLN
1	E	131	TRP
1	E	158	SER
1	E	161	HIS
1	E	168	GLU
1	E	173	ASN
1	E	174	LEU
1	E	183	ARG
1	E	208	LEU
1	E	251	CYS
1	E	261	GLN
2	F	2	GLN
2	F	4	THR
2	F	28	SER
2	F	35	ILE
2	F	38	ASP
2	F	47	GLU
2	F	81	ARG
2	F	85	VAL
2	F	89	GLN
2	F	92	ILE
2	F	97	ARG
1	G	7	LEU
1	G	8	LEU
1	G	27	SER
1	G	34	GLN
1	G	41	LEU
1	G	48	CYS
1	G	62	GLU
1	G	71	LYS
1	G	82	LEU
1	G	126	THR
1	G	131	TRP
1	G	133	GLU
1	G	140	ARG
1	G	158	SER
1	G	183	ARG

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Mol	Chain	Res	Type
1	G	221	THR
1	G	241	THR
1	G	248	HIS
2	H	51	HIS
2	H	52	SER
2	H	55	SER
2	H	64	LEU
2	H	88	SER
2	H	99	MET
3	I	13	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	173	ASN
1	A	229	ASN
1	A	256	HIS
2	B	24	ASN
1	C	91	GLN
1	C	173	ASN
1	C	256	HIS
2	D	42	ASN
1	E	34	GLN
1	E	139	GLN
1	E	142	GLN
1	E	256	HIS
2	F	2	GLN
2	F	8	GLN
2	F	42	ASN
2	F	89	GLN
1	G	139	GLN
1	G	229	ASN
2	H	31	HIS
3	J	106	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

6 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
3	MLE	I	10	3	8,8,9	6.25	1 (12%)	6,9,11	0.93	0
3	LE1	I	3	3	7,7,8	7.45	2 (28%)	8,10,12	12.99	2 (25%)
3	SAR	I	9	3	4,4,5	9.10	2 (50%)	1,3,5	1.71	0
3	LE1	J	103	3	7,7,8	6.59	2 (28%)	8,10,12	13.02	1 (12%)
3	SAR	J	109	3	4,4,5	9.46	2 (50%)	1,3,5	1.77	0
3	MLE	J	110	3	8,8,9	6.73	1 (12%)	6,9,11	1.09	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MLE	I	10	3	-	0/6/8/10	0/0/0/0
3	LE1	I	3	3	-	0/4/8/10	0/0/0/0
3	SAR	I	9	3	-	0/1/2/3	0/0/0/0
3	LE1	J	103	3	-	0/4/8/10	0/0/0/0
3	SAR	J	109	3	-	0/1/2/3	0/0/0/0
3	MLE	J	110	3	-	0/6/8/10	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	3	LE1	O-C	19.45	1.24	1.11
3	J	110	MLE	O-C	18.93	1.24	1.11
3	J	109	SAR	O-C	18.67	1.24	1.11
3	I	9	SAR	O-C	18.06	1.23	1.11
3	I	10	MLE	O-C	17.61	1.23	1.11
3	J	103	LE1	O-C	17.20	1.23	1.11
3	J	109	SAR	CA-C	2.89	1.52	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	3	LE1	CA-C	2.76	1.53	1.48
3	J	103	LE1	CA-C	2.29	1.52	1.48
3	I	9	SAR	CA-C	2.25	1.51	1.48

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	103	LE1	C-CA-N	-36.77	109.10	113.27
3	I	3	LE1	C-CA-N	-36.62	109.12	113.27
3	I	3	LE1	C8-CB-C9	-2.13	105.14	109.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	263/267 (98%)	-0.02	0 100 100	93, 107, 114, 120	0
1	C	263/267 (98%)	0.04	1 (0%) 90 45	84, 110, 127, 132	0
1	E	263/267 (98%)	-0.02	2 (0%) 83 28	87, 105, 115, 119	0
1	G	263/267 (98%)	0.03	4 (1%) 70 16	86, 112, 125, 131	0
2	B	99/99 (100%)	0.13	4 (4%) 36 5	112, 126, 145, 148	0
2	D	99/99 (100%)	0.11	0 100 100	102, 114, 136, 147	0
2	F	99/99 (100%)	0.23	4 (4%) 36 5	110, 124, 141, 142	0
2	H	99/99 (100%)	0.03	1 (1%) 79 23	94, 111, 120, 127	0
3	I	11/16 (68%)	0.47	1 (9%) 9 2	97, 100, 107, 109	0
3	J	12/16 (75%)	0.18	0 100 100	102, 109, 111, 112	0
All	All	1471/1496 (98%)	0.04	17 (1%) 75 20	84, 110, 130, 148	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	264	ARG	3.5
2	B	78	TYR	3.0
1	G	75	PHE	2.8
1	E	30	LEU	2.5
2	F	65	LEU	2.4
1	C	128	GLY	2.4
2	B	23	LEU	2.3
2	F	64	LEU	2.2
2	F	9	VAL	2.2
1	E	44	GLU	2.1
2	B	25	CYS	2.1
1	G	45	ALA	2.1
2	F	1	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	82	VAL	2.1
2	B	8	GLN	2.1
3	I	3	LE1	2.0
1	G	170	GLY	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	MLE	J	110	9/10	0.28	1.64	109,110,110,110	0
3	SAR	J	109	5/6	0.27	1.12	108,108,109,109	0
3	LE1	I	3	8/9	0.27	0.40	104,105,106,108	0
3	MLE	I	10	9/10	0.31	0.28	103,103,104,105	0
3	SAR	I	9	5/6	0.24	0.15	100,100,102,102	0
3	LE1	J	103	8/9	0.20	0.01	108,109,109,112	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.