



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 9, 2023 – 05:28 PM EDT

PDB ID : 4I18
Title : Crystal structure of human prolactin receptor complexed with Fab fragment
Authors : Duguid, E.M.; Mukherjee, S.; Kouadio, J.L.
Deposited on : 2012-11-20
Resolution : 3.24 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

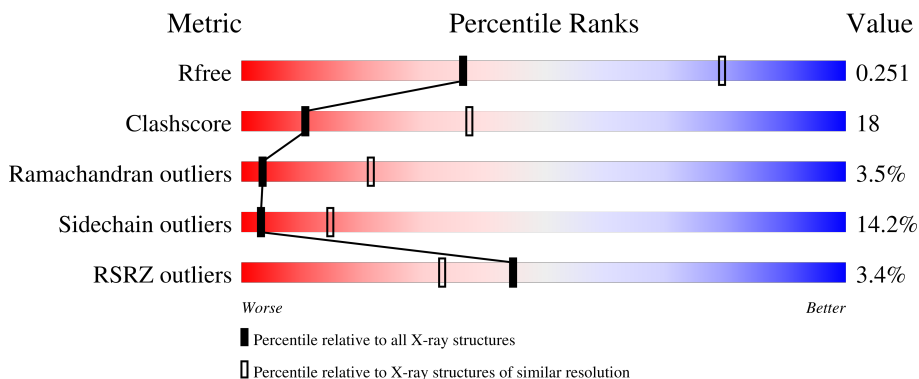
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1619 (3.28-3.20)
Clashscore	141614	1755 (3.28-3.20)
Ramachandran outliers	138981	1728 (3.28-3.20)
Sidechain outliers	138945	1727 (3.28-3.20)
RSRZ outliers	127900	1567 (3.28-3.20)

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	B	217	 2% 72% 23% . .
1	L	217	 71% 24% .
2	A	236	 3% 69% 17% 7% 7%
2	H	236	 69% 21% 6% . .
3	C	211	 10% 37% 30% 18% . 11%

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Mol	Chain	Length	Quality of chain
3	R	211	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	ACT	R	301	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9903 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 antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	216	Total 1673	C 1052	N 276	O 340	S 5	0	0	0
1	B	215	Total 1664	C 1047	N 275	O 337	S 5	0	0	0

- Molecule 2 is a protein called antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	227	Total 1686	C 1065	N 278	O 336	S 7	0	0	0
2	A	220	Total 1641	C 1039	N 270	O 325	S 7	0	0	1

- Molecule 3 is a protein called Prolactin receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	R	205	Total 1677	C 1086	N 273	O 307	S 11	0	0	0
3	C	188	Total 1532	C 999	N 246	O 278	S 9	0	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).

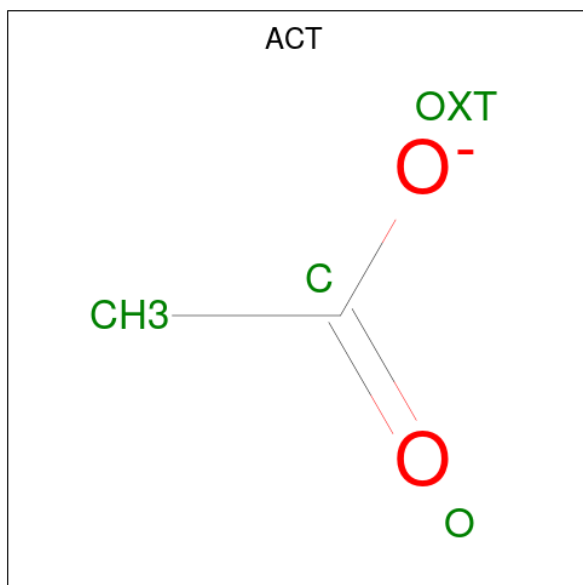


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	1	Total C O 6 3 3	0	0
4	H	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total Ca 1 1	0	0
5	B	1	Total Ca 1 1	0	0

- Molecule 6 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).

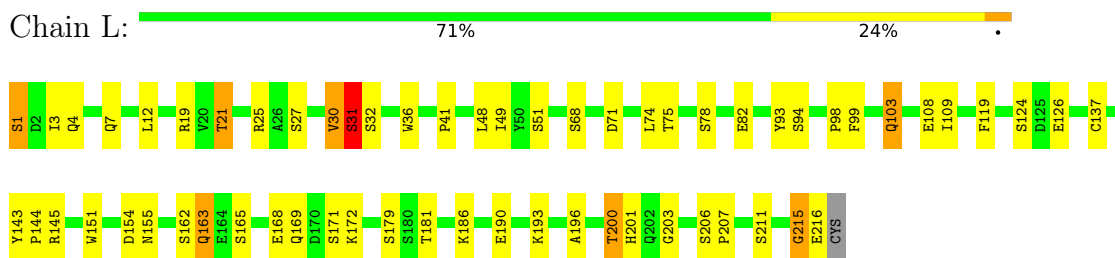


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	R	1	Total	C	O	0	0
			4	2	2		

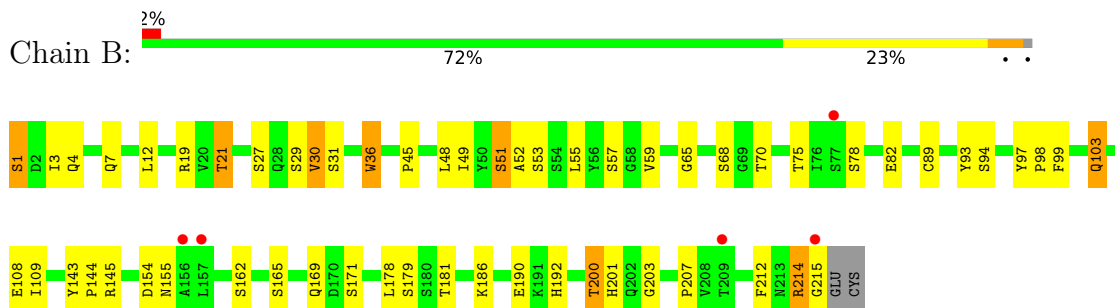
3 Residue-property plots

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.

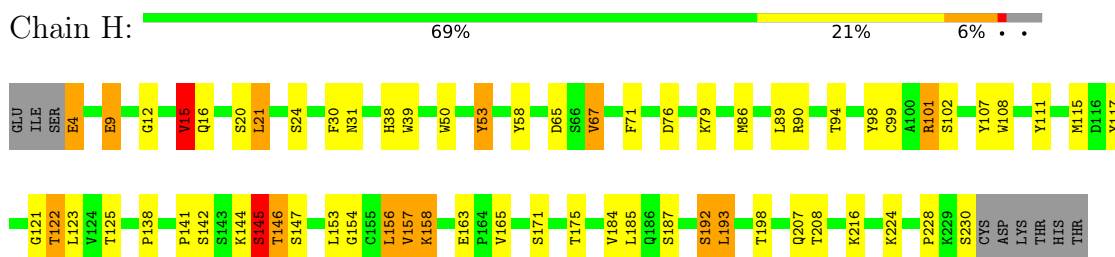
- Molecule 1: antibody light chain



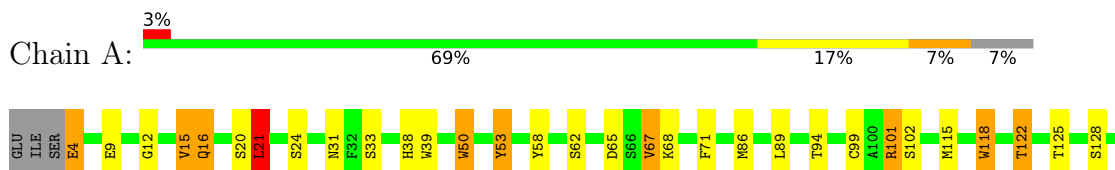
- Molecule 1: antibody light chain

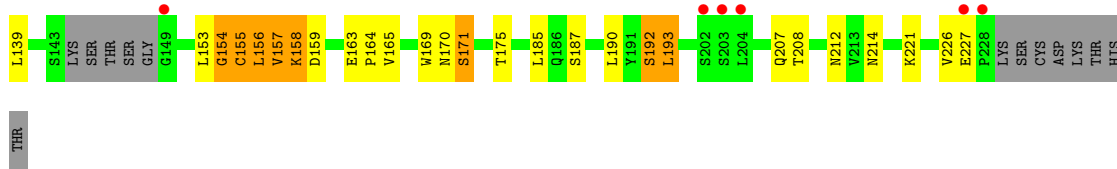


- Molecule 2: antibody heavy chain

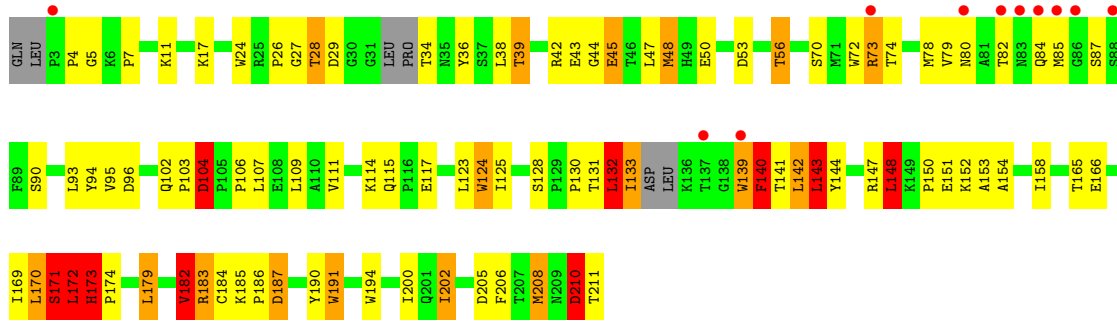


- Molecule 2: antibody heavy chain

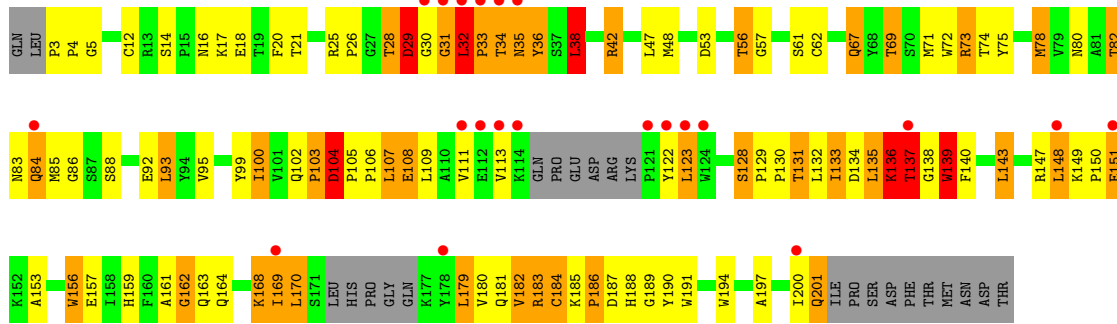




• Molecule 3: Prolactin receptor



• Molecule 3: Prolactin receptor



4 Data and refinement statistics i

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	285.83Å 285.83Å 62.25Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.51 – 3.24 49.51 – 3.24	Depositor EDS
% Data completeness (in resolution range)	99.3 (49.51-3.24) 99.4 (49.51-3.24)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 3.25Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.191 , 0.246 0.202 , 0.251	Depositor DCC
R_{free} test set	2365 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtrriage
Anisotropy	0.268	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 60.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.015 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9903	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.10% 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: ACT, CA, GOL

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	B	0.69	1/1703 (0.1%)	0.85	0/2313
1	L	0.77	0/1712	0.87	0/2325
2	A	0.92	4/1685 (0.2%)	1.01	2/2301 (0.1%)
2	H	0.90	2/1731 (0.1%)	1.07	4/2363 (0.2%)
3	C	0.91	2/1588 (0.1%)	1.06	5/2168 (0.2%)
3	R	0.98	5/1737 (0.3%)	1.13	13/2368 (0.5%)
All	All	0.87	14/10156 (0.1%)	1.00	24/13838 (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
2	A	0	2
2	H	0	1
3	C	0	3
3	R	0	1
All	All	0	7

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	191	TRP	CD2-CE2	6.02	1.48	1.41
2	A	39	TRP	CD2-CE2	5.82	1.48	1.41
2	A	50	TRP	CD2-CE2	5.58	1.48	1.41
3	R	72	TRP	CD2-CE2	5.52	1.48	1.41
3	R	124	TRP	CD2-CE2	5.50	1.48	1.41
3	C	139	TRP	CD2-CE2	5.50	1.48	1.41
3	R	139	TRP	CD2-CE2	5.47	1.48	1.41
3	C	156	TRP	CD2-CE2	5.46	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	R	24	TRP	CD2-CE2	5.33	1.47	1.41
2	A	169	TRP	CD2-CE2	5.32	1.47	1.41
1	B	36	TRP	CD2-CE2	5.29	1.47	1.41
2	A	118	TRP	CD2-CE2	5.21	1.47	1.41
2	H	39	TRP	CD2-CE2	5.16	1.47	1.41
2	H	108	TRP	CD2-CE2	5.03	1.47	1.41

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	R	132	LEU	CA-CB-CG	7.41	132.33	115.30
2	A	21	LEU	CB-CG-CD1	-7.25	98.67	111.00
3	R	104	ASP	CB-CG-OD2	-7.16	111.85	118.30
2	H	156	LEU	C-N-CA	7.12	139.51	121.70
2	A	156	LEU	C-N-CA	7.08	139.41	121.70
2	H	156	LEU	N-CA-C	-6.83	92.55	111.00
3	C	38	LEU	CA-CB-CG	6.80	130.94	115.30
3	R	182	VAL	CB-CA-C	-6.16	99.69	111.40
3	R	143	LEU	CA-CB-CG	-6.15	101.15	115.30
3	R	210	ASP	N-CA-C	6.13	127.55	111.00
3	R	104	ASP	CB-CG-OD1	6.10	123.79	118.30
3	C	104	ASP	N-CA-CB	-5.98	99.84	110.60
2	H	15	VAL	CB-CA-C	-5.96	100.07	111.40
3	R	45	GLU	N-CA-C	-5.87	95.15	111.00
3	C	104	ASP	CB-CG-OD1	5.74	123.47	118.30
3	R	172	LEU	N-CA-C	-5.56	95.98	111.00
3	R	140	PHE	N-CA-C	5.53	125.94	111.00
3	C	104	ASP	CB-CG-OD2	-5.50	113.35	118.30
3	R	148	LEU	CA-CB-CG	5.41	127.75	115.30
3	R	96	ASP	CB-CG-OD1	5.23	123.01	118.30
3	R	114	LYS	CD-CE-NZ	5.21	123.69	111.70
3	R	104	ASP	N-CA-CB	-5.13	101.36	110.60
2	H	145	SER	N-CA-C	5.10	124.76	111.00
3	C	136	LYS	N-CA-C	-5.01	97.47	111.00

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	154	GLY	Peptide
2	A	155	CYS	Peptide
3	C	103	PRO	Peptide

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Mol	Chain	Res	Type	Group
3	C	136	LYS	Peptide
3	C	35	ASN	Peptide
2	H	154	GLY	Peptide
3	R	103	PRO	Peptide

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	B	1664	0	1610	41	0
1	L	1673	0	1616	45	0
2	A	1641	0	1567	50	0
2	H	1686	0	1605	58	0
3	C	1532	0	1446	110	0
3	R	1677	0	1586	83	0
4	A	6	0	8	0	0
4	C	6	0	8	0	0
4	H	6	0	8	2	0
4	L	6	0	8	0	0
5	B	1	0	0	0	0
5	H	1	0	0	0	0
6	R	4	0	3	2	0
All	All	9903	0	9465	358	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 18.

All (358) 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)
3:R:172:LEU:CA	3:R:173:HIS:HB2	1.69	1.20
3:C:30:GLY:HA2	3:C:31:GLY:O	1.43	1.17
1:L:119:PHE:CD1	2:H:145:SER:HA	1.81	1.16
3:R:170:LEU:O	3:R:171:SER:HB2	1.43	1.15
3:R:172:LEU:O	3:R:172:LEU:HD12	1.50	1.09
2:A:16:GLN:HA	2:A:16:GLN:HE21	1.09	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:119:PHE:HD1	2:H:145:SER:HA	1.04	1.07
3:R:82:THR:HA	3:R:87:SER:HB3	1.31	1.07
3:R:172:LEU:HA	3:R:173:HIS:CB	1.86	1.06
3:R:53:ASP:OD2	3:R:56:THR:HG23	1.63	0.99
3:R:11:LYS:CE	6:R:301:ACT:H2	1.93	0.98
3:R:111:VAL:HG12	3:R:200:ILE:HD13	1.47	0.95
1:B:190:GLU:HA	1:B:214:ARG:HD2	1.45	0.95
3:C:26:PRO:HB3	3:C:36:TYR:OH	1.65	0.94
2:A:16:GLN:HA	2:A:16:GLN:NE2	1.81	0.94
3:R:172:LEU:HA	3:R:173:HIS:HB2	0.93	0.93
3:R:104:ASP:HB3	3:R:130:PRO:HB3	1.51	0.91
3:C:35:ASN:HA	3:C:36:TYR:HB2	1.54	0.90
3:R:172:LEU:HD13	3:R:202:ILE:HD12	1.56	0.87
3:C:103:PRO:HB3	3:C:133:ILE:HD12	1.56	0.87
2:H:4:GLU:OE2	2:H:4:GLU:HA	1.73	0.87
3:R:171:SER:O	3:R:172:LEU:HG	1.75	0.87
3:C:32:LEU:HB3	3:C:33:PRO:HD2	1.57	0.86
2:H:15:VAL:CG2	2:H:21:LEU:HD13	2.09	0.82
3:C:28:THR:HG22	3:C:28:THR:O	1.80	0.81
2:A:38:HIS:CD2	2:A:115:MET:HE1	2.15	0.81
1:L:163:GLN:HG2	2:H:184:VAL:HG11	1.61	0.81
3:R:53:ASP:OD2	3:R:56:THR:CG2	2.28	0.81
3:R:47:LEU:O	3:R:48:MET:HB2	1.80	0.81
3:R:171:SER:O	3:R:172:LEU:CG	2.29	0.81
2:H:15:VAL:HG21	2:H:21:LEU:HD13	1.64	0.80
3:R:5:GLY:HA2	3:R:28:THR:HB	1.63	0.80
3:C:4:PRO:HD3	3:C:83:ASN:HD22	1.46	0.80
3:R:148:LEU:HD21	3:R:169:ILE:HD13	1.64	0.79
1:L:109:ILE:HB	1:L:169:GLN:HE22	1.48	0.79
1:L:201:HIS:CD2	1:L:203:GLY:H	2.01	0.79
3:R:171:SER:O	3:R:172:LEU:CB	2.31	0.78
1:B:214:ARG:HG2	1:B:215:GLY:N	1.98	0.78
3:R:172:LEU:HD12	3:R:172:LEU:C	2.03	0.78
3:R:172:LEU:O	3:R:172:LEU:CD1	2.30	0.77
2:A:16:GLN:HE21	2:A:16:GLN:CA	1.92	0.76
3:C:169:ILE:C	3:C:170:LEU:HG	2.06	0.76
3:R:53:ASP:CG	3:R:56:THR:HG23	2.06	0.75
3:R:170:LEU:O	3:R:171:SER:CB	2.29	0.74
3:C:32:LEU:HD13	3:C:84:GLN:HG2	1.67	0.74
2:H:207:GLN:HE21	2:H:208:THR:N	1.85	0.73
2:H:31:ASN:H	3:C:56:THR:HG21	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:53:ASP:OD1	3:C:56:THR:HG23	1.88	0.73
3:C:30:GLY:HA2	3:C:31:GLY:C	2.08	0.72
1:L:7:GLN:H	1:L:103:GLN:HE22	1.39	0.71
1:L:21:THR:O	1:L:21:THR:HG22	1.91	0.71
3:R:171:SER:C	3:R:172:LEU:HG	2.11	0.71
3:C:34:THR:CG2	3:C:83:ASN:HB2	2.20	0.71
1:B:109:ILE:HB	1:B:169:GLN:HE22	1.56	0.70
3:C:32:LEU:HB3	3:C:33:PRO:CD	2.21	0.69
1:L:108:GLU:HG2	1:L:169:GLN:OE1	1.92	0.69
3:C:28:THR:O	3:C:28:THR:CG2	2.41	0.68
1:B:192:HIS:O	1:B:214:ARG:HD3	1.94	0.68
3:R:143:LEU:O	3:R:184:CYS:HB2	1.93	0.68
2:A:207:GLN:HE21	2:A:208:THR:N	1.92	0.67
2:A:101:ARG:HD3	2:A:101:ARG:C	2.14	0.67
2:A:4:GLU:OE2	2:A:4:GLU:HA	1.94	0.67
3:C:143:LEU:HA	3:C:162:GLY:O	1.94	0.67
3:R:132:LEU:O	3:R:133:ILE:HB	1.95	0.66
3:C:35:ASN:HA	3:C:36:TYR:CB	2.25	0.66
3:C:4:PRO:HD3	3:C:83:ASN:ND2	2.11	0.66
1:B:201:HIS:CD2	1:B:203:GLY:H	2.13	0.65
2:H:15:VAL:HG22	2:H:21:LEU:CD1	2.26	0.65
3:R:171:SER:O	3:R:172:LEU:HB3	1.94	0.65
3:C:131:THR:O	3:C:132:LEU:HB2	1.95	0.65
3:C:183:ARG:HG3	3:C:191:TRP:CE3	2.31	0.65
3:C:3:PRO:HA	3:C:86:GLY:HA3	1.78	0.65
2:H:38:HIS:CD2	2:H:53:TYR:HB3	2.31	0.65
3:C:148:LEU:CD1	3:C:157:GLU:HB3	2.27	0.65
3:C:42:ARG:HH21	3:C:74:THR:H	1.44	0.65
1:L:30:VAL:HG22	1:L:93:TYR:HB3	1.79	0.65
1:B:214:ARG:CG	1:B:215:GLY:N	2.59	0.64
2:A:38:HIS:CD2	2:A:50:TRP:HE1	2.16	0.64
3:C:35:ASN:HA	3:C:36:TYR:CD2	2.32	0.64
1:B:200:THR:HG23	1:B:207:PRO:HG3	1.80	0.64
2:A:58:TYR:CE1	3:R:132:LEU:HA	2.32	0.64
1:L:119:PHE:HD1	2:H:145:SER:CA	1.96	0.64
1:B:21:THR:HG22	1:B:21:THR:O	1.97	0.64
2:H:38:HIS:CD2	2:H:50:TRP:HE1	2.15	0.64
2:H:144:LYS:HA	2:H:146:THR:H	1.62	0.63
3:C:201:GLN:C	3:C:201:GLN:NE2	2.52	0.63
2:H:9:GLU:OE2	2:H:99:CYS:N	2.29	0.63
3:C:35:ASN:HA	3:C:36:TYR:HD2	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:PRO:HG2	2:A:118:TRP:CZ3	2.33	0.63
1:L:31:SER:OG	1:L:32:SER:N	2.25	0.62
3:C:102:GLN:HB2	3:C:190:TYR:HB2	1.82	0.62
1:B:30:VAL:HG22	1:B:93:TYR:HB3	1.82	0.62
1:L:200:THR:HG23	1:L:207:PRO:HG3	1.82	0.62
3:C:53:ASP:CG	3:C:56:THR:HG23	2.20	0.62
3:C:169:ILE:HG23	3:C:170:LEU:N	2.15	0.61
2:A:94:THR:HG23	2:A:125:THR:HA	1.81	0.61
2:A:38:HIS:HD2	2:A:50:TRP:HE1	1.47	0.61
3:C:53:ASP:OD2	3:C:56:THR:HG23	2.00	0.61
2:H:15:VAL:CG2	2:H:21:LEU:CD1	2.78	0.61
3:C:18:GLU:HA	3:C:69:THR:HG21	1.81	0.61
2:H:31:ASN:H	3:C:56:THR:CG2	2.13	0.61
3:C:35:ASN:CA	3:C:36:TYR:HB2	2.30	0.60
1:L:7:GLN:H	1:L:103:GLN:NE2	1.99	0.60
3:C:42:ARG:NH2	3:C:74:THR:H	1.98	0.60
3:C:106:PRO:HG2	3:C:182:VAL:HB	1.84	0.60
3:C:35:ASN:CA	3:C:36:TYR:HD2	2.14	0.60
2:H:101:ARG:HD3	2:H:101:ARG:C	2.22	0.60
1:L:186:LYS:HE2	1:L:190:GLU:OE2	2.02	0.60
2:H:38:HIS:HD2	2:H:50:TRP:HE1	1.49	0.60
1:L:154:ASP:O	1:L:155:ASN:HB2	2.02	0.59
2:A:214:ASN:HD21	2:A:221:LYS:HE2	1.67	0.59
3:C:78:MET:HG3	3:C:92:GLU:HG2	1.84	0.59
3:R:172:LEU:CA	3:R:173:HIS:CB	2.57	0.59
3:R:142:LEU:HD12	3:R:186:PRO:HA	1.84	0.58
3:C:99:TYR:HD2	3:C:188:HIS:HB2	1.68	0.58
2:H:38:HIS:CD2	2:H:115:MET:HE1	2.37	0.58
3:C:34:THR:HG22	3:C:83:ASN:HB2	1.84	0.58
3:C:148:LEU:HA	3:C:179:LEU:O	2.02	0.58
3:C:168:LYS:H	3:C:168:LYS:HD3	1.68	0.58
1:B:143:TYR:CD1	1:B:144:PRO:HA	2.39	0.58
2:A:15:VAL:HG21	2:A:21:LEU:HD13	1.85	0.58
2:H:9:GLU:OE2	2:H:98:TYR:HA	2.03	0.58
1:B:98:PRO:HB2	1:B:99:PHE:CD2	2.38	0.58
2:H:107:TYR:O	4:H:302:GOL:H32	2.03	0.58
1:L:124:SER:CB	2:H:138:PRO:HD2	2.34	0.58
3:C:169:ILE:O	3:C:170:LEU:HG	2.03	0.58
3:C:184:CYS:HA	3:C:191:TRP:HZ3	1.68	0.58
2:H:16:GLN:HA	2:H:16:GLN:NE2	2.19	0.57
3:C:168:LYS:HD3	3:C:168:LYS:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:183:ARG:HD2	3:R:194:TRP:CZ3	2.40	0.57
3:C:113:VAL:HG23	3:C:200:ILE:HD11	1.86	0.57
3:R:169:ILE:HG21	3:R:172:LEU:HD23	1.87	0.57
2:A:38:HIS:CD2	2:A:53:TYR:HB3	2.40	0.57
3:C:99:TYR:CD2	3:C:188:HIS:HB2	2.39	0.57
1:L:215:GLY:O	1:L:216:GLU:HG3	2.04	0.56
2:H:38:HIS:HE1	2:H:102:SER:HB3	1.70	0.56
2:H:76:ASP:OD2	2:H:79:LYS:HD2	2.05	0.56
2:A:139:LEU:HD12	2:A:154:GLY:HA3	1.87	0.56
3:C:83:ASN:O	3:C:84:GLN:HB2	2.04	0.56
3:C:128:SER:HB2	3:C:129:PRO:HD2	1.86	0.56
2:H:144:LYS:HA	2:H:146:THR:N	2.20	0.56
3:C:169:ILE:CG2	3:C:170:LEU:N	2.69	0.56
3:R:94:TYR:N	3:R:94:TYR:CD1	2.74	0.56
3:R:124:TRP:CH2	3:R:166:GLU:OE1	2.58	0.56
1:L:4:GLN:HB2	1:L:27:SER:HB3	1.88	0.56
2:A:9:GLU:HA	2:A:24:SER:O	2.06	0.56
2:A:31:ASN:H	3:R:56:THR:CG2	2.18	0.56
2:A:16:GLN:HE22	2:A:128:SER:HA	1.69	0.56
2:H:193:LEU:C	2:H:193:LEU:HD12	2.26	0.56
1:L:99:PHE:HB3	2:H:115:MET:HE3	1.88	0.55
3:C:134:ASP:O	3:C:135:LEU:HD12	2.06	0.55
1:L:201:HIS:HD2	1:L:203:GLY:H	1.53	0.55
3:R:104:ASP:HB3	3:R:130:PRO:CB	2.32	0.55
3:C:57:GLY:HA3	3:C:61:SER:OG	2.06	0.55
3:R:111:VAL:CG1	3:R:200:ILE:HD13	2.29	0.55
2:A:38:HIS:CD2	2:A:115:MET:CE	2.90	0.54
3:C:93:LEU:HD23	3:C:95:VAL:HG22	1.89	0.54
3:C:4:PRO:HB3	3:C:5:GLY:HA3	1.90	0.54
1:B:53:SER:HB2	1:B:65:GLY:O	2.07	0.54
2:A:101:ARG:NH2	3:R:56:THR:O	2.32	0.54
1:L:124:SER:HB3	2:H:138:PRO:HD2	1.89	0.54
3:C:16:ASN:ND2	3:C:18:GLU:HB2	2.22	0.54
2:A:16:GLN:NE2	2:A:16:GLN:CA	2.58	0.54
1:L:163:GLN:CG	2:H:184:VAL:HG11	2.35	0.54
2:H:101:ARG:HD2	2:H:117:TYR:HD2	1.73	0.54
3:R:111:VAL:HG12	3:R:200:ILE:CD1	2.32	0.54
3:R:172:LEU:CD1	3:R:202:ILE:HD12	2.34	0.54
3:R:94:TYR:N	3:R:94:TYR:HD1	2.05	0.54
2:H:58:TYR:CE2	3:C:132:LEU:CD2	2.92	0.53
3:C:33:PRO:O	3:C:34:THR:HG23	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:179:LEU:HD23	3:C:197:ALA:HB1	1.89	0.53
3:R:131:THR:O	3:R:132:LEU:HG	2.09	0.53
2:H:141:PRO:HG2	2:H:228:PRO:HB3	1.89	0.53
2:A:15:VAL:CG2	2:A:21:LEU:HD13	2.38	0.53
2:A:207:GLN:HE21	2:A:208:THR:H	1.54	0.53
1:B:99:PHE:HB3	2:A:115:MET:HE3	1.90	0.53
3:C:74:THR:C	3:C:75:TYR:CD2	2.83	0.53
3:C:107:LEU:HD13	3:C:108:GLU:H	1.74	0.53
3:R:183:ARG:HD2	3:R:194:TRP:CH2	2.44	0.52
1:B:214:ARG:CG	1:B:215:GLY:H	2.22	0.52
3:R:53:ASP:OD1	3:R:56:THR:HG23	2.09	0.52
3:C:16:ASN:HD21	3:C:18:GLU:HB2	1.75	0.52
3:R:172:LEU:C	3:R:172:LEU:CD1	2.73	0.52
1:B:3:ILE:HD12	1:B:94:SER:HB2	1.91	0.52
2:A:38:HIS:HE1	2:A:102:SER:HB3	1.74	0.52
3:C:48:MET:HE2	3:C:78:MET:HE2	1.92	0.52
3:C:103:PRO:HB3	3:C:133:ILE:CD1	2.32	0.52
3:C:184:CYS:HA	3:C:191:TRP:CZ3	2.44	0.52
3:C:150:PRO:HB2	3:C:153:ALA:HB2	1.91	0.52
2:H:30:PHE:CZ	2:H:101:ARG:HG2	2.45	0.51
3:R:147:ARG:HD3	3:R:194:TRP:CZ2	2.45	0.51
2:A:139:LEU:HB2	2:A:154:GLY:HA3	1.91	0.51
1:L:25:ARG:HG3	1:L:71:ASP:OD1	2.11	0.51
2:H:58:TYR:CE2	3:C:132:LEU:HD22	2.45	0.51
3:C:148:LEU:HD12	3:C:157:GLU:HB3	1.92	0.51
3:R:107:LEU:HD11	3:R:131:THR:CG2	2.41	0.51
3:R:115:GLN:HE22	3:R:208:MET:CE	2.24	0.51
3:R:172:LEU:O	3:R:172:LEU:CG	2.59	0.51
1:L:1:SER:HB2	1:L:4:GLN:HE22	1.75	0.51
2:A:163:GLU:HB3	2:A:164:PRO:HA	1.93	0.51
3:C:109:LEU:HD13	3:C:182:VAL:HG22	1.92	0.51
2:A:31:ASN:H	3:R:56:THR:HG21	1.75	0.50
3:R:179:LEU:H	3:R:179:LEU:HD12	1.75	0.50
1:L:21:THR:O	1:L:21:THR:CG2	2.55	0.50
2:A:4:GLU:OE2	2:A:4:GLU:CA	2.60	0.50
3:R:169:ILE:CG2	3:R:172:LEU:HD23	2.42	0.50
3:R:5:GLY:CA	3:R:28:THR:HB	2.39	0.50
3:C:28:THR:O	3:C:29:ASP:C	2.50	0.50
3:C:201:GLN:C	3:C:201:GLN:HE21	2.14	0.50
3:C:104:ASP:O	3:C:130:PRO:HB3	2.12	0.50
3:C:123:LEU:HD21	3:C:200:ILE:HD13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ASP:O	1:B:155:ASN:HB2	2.12	0.50
2:A:86:MET:HB3	2:A:89:LEU:HD21	1.94	0.50
1:L:196:ALA:HB2	1:L:211:SER:HB3	1.94	0.50
1:B:7:GLN:H	1:B:103:GLN:NE2	2.09	0.50
3:R:39:THR:HG22	3:R:50:GLU:HA	1.93	0.49
2:A:31:ASN:HB2	3:R:56:THR:HG21	1.95	0.49
3:C:169:ILE:HG23	3:C:170:LEU:H	1.76	0.49
1:B:55:LEU:HD11	1:B:59:VAL:CG1	2.43	0.49
1:B:186:LYS:HE2	1:B:190:GLU:OE2	2.13	0.49
2:A:67:VAL:HG13	2:A:71:PHE:HB2	1.94	0.49
3:C:73:ARG:HB3	3:C:73:ARG:CZ	2.43	0.49
2:A:31:ASN:CB	3:R:56:THR:HG21	2.43	0.49
1:L:82:GLU:HA	1:L:171:SER:HB2	1.95	0.48
2:H:38:HIS:O	2:H:99:CYS:HA	2.13	0.48
3:C:14:SER:HB2	3:C:20:PHE:HB3	1.96	0.48
1:L:143:TYR:CD1	1:L:144:PRO:HA	2.49	0.48
3:C:159:HIS:CD2	3:C:169:ILE:HD11	2.48	0.48
2:H:207:GLN:NE2	2:H:208:THR:N	2.59	0.48
3:C:71:MET:HG3	3:C:72:TRP:H	1.78	0.48
3:C:186:PRO:O	3:C:187:ASP:C	2.52	0.48
2:H:16:GLN:HA	2:H:16:GLN:HE21	1.79	0.48
1:B:82:GLU:HA	1:B:171:SER:HB2	1.96	0.48
1:B:108:GLU:HG2	1:B:169:GLN:OE1	2.14	0.48
3:C:104:ASP:OD2	3:C:131:THR:O	2.32	0.47
1:B:55:LEU:HD11	1:B:59:VAL:HG12	1.96	0.47
2:H:94:THR:HG23	2:H:125:THR:HA	1.95	0.47
3:C:161:ALA:O	3:C:163:GLN:N	2.48	0.47
3:C:111:VAL:HG12	3:C:200:ILE:HD12	1.97	0.47
1:B:97:TYR:N	1:B:98:PRO:CD	2.78	0.47
1:L:143:TYR:CG	1:L:144:PRO:HA	2.50	0.47
1:B:36:TRP:CH2	1:B:89:CYS:HB3	2.50	0.47
3:C:107:LEU:HD22	3:C:107:LEU:HA	1.62	0.47
2:H:158:LYS:HG2	2:H:192:SER:OG	2.16	0.46
2:A:139:LEU:HB2	2:A:154:GLY:CA	2.44	0.46
3:R:173:HIS:H	3:R:174:PRO:HD3	1.80	0.46
3:R:174:PRO:HA	3:R:202:ILE:HG22	1.96	0.46
2:H:4:GLU:OE2	2:H:4:GLU:CA	2.57	0.46
3:C:42:ARG:NH2	3:C:73:ARG:H	2.13	0.46
3:C:113:VAL:CG2	3:C:200:ILE:HD11	2.44	0.46
3:C:21:THR:HG23	3:C:62:CYS:O	2.15	0.46
3:C:32:LEU:HD22	3:C:84:GLN:OE1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:32:LEU:HD13	3:C:84:GLN:CG	2.41	0.46
3:C:4:PRO:CB	3:C:5:GLY:HA3	2.46	0.46
1:B:21:THR:O	1:B:21:THR:CG2	2.61	0.46
2:A:50:TRP:HE1	2:A:115:MET:HE1	1.81	0.46
3:R:150:PRO:HG2	3:R:153:ALA:HB2	1.97	0.46
3:R:173:HIS:H	3:R:174:PRO:CD	2.27	0.46
3:C:106:PRO:CG	3:C:182:VAL:HB	2.45	0.46
2:H:9:GLU:OE1	2:H:121:GLY:N	2.37	0.46
1:L:99:PHE:CG	2:H:115:MET:HE3	2.51	0.46
3:C:151:GLU:HA	3:C:179:LEU:HD12	1.98	0.46
1:L:30:VAL:HG22	1:L:93:TYR:CB	2.46	0.45
1:B:51:SER:O	1:B:52:ALA:HB3	2.16	0.45
3:R:34:THR:HG22	3:R:36:TYR:CE2	2.51	0.45
3:C:35:ASN:CA	3:C:36:TYR:CD2	2.95	0.45
3:C:53:ASP:OD2	3:C:56:THR:CG2	2.63	0.45
1:B:143:TYR:CG	1:B:144:PRO:HA	2.51	0.45
3:C:137:THR:CG2	3:C:139:TRP:CE3	2.99	0.45
1:B:7:GLN:H	1:B:103:GLN:HE22	1.65	0.45
2:A:12:GLY:HA3	2:A:122:THR:HB	1.99	0.45
2:A:158:LYS:HD3	2:A:159:ASP:OD1	2.17	0.45
3:R:107:LEU:HD11	3:R:131:THR:HG23	1.97	0.45
1:B:53:SER:CB	1:B:65:GLY:O	2.65	0.45
2:H:38:HIS:CD2	2:H:115:MET:CE	2.99	0.45
2:H:50:TRP:HE1	2:H:115:MET:HE1	1.82	0.44
3:R:7:PRO:HG2	3:R:90:SER:HB3	1.98	0.44
3:R:139:TRP:CG	3:R:140:PHE:N	2.84	0.44
3:C:38:LEU:HD12	3:C:38:LEU:C	2.38	0.44
3:C:183:ARG:HD2	3:C:194:TRP:CE2	2.52	0.44
2:A:58:TYR:CE2	3:R:132:LEU:HD22	2.53	0.44
3:C:67:GLN:HE21	3:C:67:GLN:HB3	1.64	0.44
2:A:158:LYS:HA	2:A:192:SER:OG	2.18	0.44
2:A:65:ASP:C	2:A:67:VAL:H	2.21	0.44
2:H:12:GLY:HA3	2:H:122:THR:HB	2.00	0.44
2:H:65:ASP:C	2:H:67:VAL:H	2.21	0.44
3:R:102:GLN:HB2	3:R:190:TYR:HB2	1.99	0.44
2:H:123:LEU:HD21	2:H:163:GLU:HB2	2.00	0.43
3:R:185:LYS:HB3	3:R:191:TRP:HA	2.00	0.43
1:L:119:PHE:HE1	2:H:146:THR:N	2.15	0.43
3:C:107:LEU:O	3:C:108:GLU:C	2.57	0.43
1:L:137:CYS:HB2	1:L:151:TRP:CH2	2.54	0.43
2:A:214:ASN:ND2	2:A:221:LYS:HG3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67:GLN:HG2	3:C:67:GLN:O	2.19	0.43
1:L:144:PRO:O	1:L:201:HIS:HE1	2.00	0.43
2:A:207:GLN:NE2	2:A:208:THR:H	2.16	0.43
1:L:215:GLY:O	1:L:216:GLU:CG	2.66	0.43
2:H:207:GLN:HE21	2:H:208:THR:H	1.65	0.43
2:H:31:ASN:N	3:C:56:THR:HG21	2.27	0.43
2:H:67:VAL:HG13	2:H:71:PHE:HB2	1.99	0.43
3:C:12:CYS:HB3	3:C:100:ILE:HD12	2.01	0.43
3:C:35:ASN:CA	3:C:36:TYR:CB	2.96	0.43
3:C:137:THR:HA	3:C:138:GLY:C	2.35	0.43
1:L:98:PRO:HB2	1:L:99:PHE:CD2	2.53	0.43
3:R:132:LEU:O	3:R:133:ILE:CB	2.66	0.43
3:C:34:THR:HG22	3:C:82:THR:O	2.19	0.43
1:L:36:TRP:CD2	1:L:74:LEU:HB2	2.53	0.42
1:B:45:PRO:HG2	2:A:118:TRP:CH2	2.54	0.42
2:A:38:HIS:O	2:A:99:CYS:HA	2.18	0.42
3:R:11:LYS:CE	6:R:301:ACT:CH3	2.82	0.42
1:B:1:SER:HA	1:B:97:TYR:CG	2.54	0.42
2:A:38:HIS:CE1	2:A:102:SER:HB3	2.54	0.42
1:L:25:ARG:NH1	1:L:25:ARG:HB2	2.35	0.42
1:B:212:PHE:CD1	1:B:212:PHE:C	2.92	0.42
3:R:106:PRO:HG2	3:R:182:VAL:HB	2.00	0.42
3:R:93:LEU:HD23	3:R:95:VAL:CG2	2.49	0.42
2:A:193:LEU:C	2:A:193:LEU:HD12	2.39	0.42
4:H:302:GOL:H12	3:C:105:PRO:HD3	2.01	0.42
1:B:4:GLN:HB2	1:B:27:SER:HB3	2.01	0.42
1:B:29:SER:HA	1:B:70:THR:HG22	2.01	0.42
3:R:125:ILE:O	3:R:166:GLU:HA	2.20	0.42
2:A:159:ASP:HB3	2:A:190:LEU:CD1	2.49	0.42
1:B:178:LEU:C	1:B:178:LEU:HD23	2.40	0.42
3:R:183:ARG:HB3	3:R:194:TRP:CE3	2.55	0.42
1:B:162:SER:HA	1:B:181:THR:O	2.19	0.41
3:R:38:LEU:HD12	3:R:79:VAL:HG22	2.02	0.41
1:L:126:GLU:OE1	2:H:224:LYS:NZ	2.54	0.41
2:H:86:MET:HB3	2:H:89:LEU:HD21	2.02	0.41
1:L:3:ILE:HD12	1:L:94:SER:HB2	2.02	0.41
1:L:41:PRO:CG	1:L:168:GLU:HG3	2.50	0.41
3:R:111:VAL:HG11	3:R:200:ILE:HG21	2.01	0.41
3:R:205:ASP:O	3:R:208:MET:HB3	2.20	0.41
1:L:99:PHE:CD1	2:H:115:MET:HE3	2.55	0.41
3:R:93:LEU:HD23	3:R:95:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:147:ARG:HB2	3:C:156:TRP:CE3	2.56	0.41
1:B:36:TRP:CZ3	1:B:89:CYS:HB3	2.55	0.41
2:H:111:TYR:OH	3:C:102:GLN:OE1	2.22	0.41
3:R:144:TYR:CD1	3:R:184:CYS:HB3	2.56	0.41
1:L:119:PHE:CE1	2:H:145:SER:HA	2.46	0.41
1:B:30:VAL:O	1:B:30:VAL:HG13	2.21	0.41
1:B:48:LEU:O	1:B:49:ILE:HG13	2.21	0.41
2:A:170:ASN:O	2:A:171:SER:C	2.59	0.41
3:C:71:MET:CG	3:C:72:TRP:H	2.33	0.41
3:C:137:THR:HG21	3:C:139:TRP:CE3	2.56	0.41
3:C:185:LYS:HD2	3:C:189:GLY:O	2.21	0.41
3:R:109:LEU:HD13	3:R:182:VAL:HG22	2.02	0.41
2:H:142:SER:O	2:H:145:SER:O	2.39	0.40
3:R:150:PRO:O	3:R:152:LYS:N	2.53	0.40
2:A:38:HIS:CG	2:A:115:MET:HE1	2.55	0.40
3:R:42:ARG:NH2	3:R:73:ARG:HG3	2.37	0.40
3:R:186:PRO:O	3:R:187:ASP:C	2.59	0.40
3:C:181:GLN:HG2	3:C:197:ALA:HA	2.02	0.40
1:L:48:LEU:O	1:L:49:ILE:HG13	2.21	0.40
3:R:26:PRO:HB3	3:R:36:TYR:CE1	2.56	0.40
3:C:17:LYS:NZ	3:C:139:TRP:O	2.54	0.40
1:L:162:SER:HA	1:L:181:THR:O	2.21	0.40
1:B:30:VAL:HG22	1:B:93:TYR:CB	2.49	0.40
3:R:125:ILE:CD1	3:R:169:ILE:HD12	2.52	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	B	213/217 (98%)	201 (94%)	10 (5%)	2 (1%)	17 52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	214/217 (99%)	201 (94%)	11 (5%)	2 (1%)	17	52
2	A	216/236 (92%)	199 (92%)	15 (7%)	2 (1%)	17	52
2	H	225/236 (95%)	207 (92%)	14 (6%)	4 (2%)	8	38
3	C	182/211 (86%)	148 (81%)	18 (10%)	16 (9%)	1	4
3	R	199/211 (94%)	159 (80%)	22 (11%)	18 (9%)	1	4
All	All	1249/1328 (94%)	1115 (89%)	90 (7%)	44 (4%)	3	21

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	145	SER
1	B	214	ARG
3	R	27	GLY
3	R	29	ASP
3	R	45	GLU
3	R	104	ASP
3	R	117	GLU
3	R	151	GLU
3	R	154	ALA
3	R	171	SER
3	R	173	HIS
3	C	29	ASP
3	C	31	GLY
3	C	32	LEU
3	C	84	GLN
1	B	31	SER
2	A	171	SER
3	R	43	GLU
3	R	44	GLY
3	R	48	MET
3	R	140	PHE
3	R	172	LEU
3	R	187	ASP
3	R	210	ASP
3	C	85	MET
3	C	136	LYS
3	C	149	LYS
3	C	162	GLY
2	H	171	SER
3	R	4	PRO

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Mol	Chain	Res	Type
3	R	206	PHE
3	C	28	THR
3	C	33	PRO
3	C	108	GLU
3	C	137	THR
2	H	146	THR
3	C	36	TYR
3	C	69	THR
3	C	186	PRO
1	L	31	SER
1	L	215	GLY
2	H	157	VAL
3	C	104	ASP
2	A	157	VAL

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	B	190/192 (99%)	175 (92%)	15 (8%)	12	40
1	L	191/192 (100%)	172 (90%)	19 (10%)	8	29
2	A	181/197 (92%)	155 (86%)	26 (14%)	3	14
2	H	185/197 (94%)	160 (86%)	25 (14%)	4	16
3	C	165/191 (86%)	126 (76%)	39 (24%)	1	3
3	R	183/191 (96%)	151 (82%)	32 (18%)	2	8
All	All	1095/1160 (94%)	939 (86%)	156 (14%)	3	15

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	SER
1	L	12	LEU
1	L	19	ARG
1	L	21	THR

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Mol	Chain	Res	Type
1	L	30	VAL
1	L	31	SER
1	L	51	SER
1	L	68	SER
1	L	75	THR
1	L	78	SER
1	L	103	GLN
1	L	145	ARG
1	L	163	GLN
1	L	165	SER
1	L	172	LYS
1	L	179	SER
1	L	193	LYS
1	L	200	THR
1	L	206	SER
2	H	4	GLU
2	H	9	GLU
2	H	15	VAL
2	H	20	SER
2	H	21	LEU
2	H	24	SER
2	H	53	TYR
2	H	67	VAL
2	H	90	ARG
2	H	101	ARG
2	H	122	THR
2	H	147	SER
2	H	153	LEU
2	H	156	LEU
2	H	157	VAL
2	H	158	LYS
2	H	165	VAL
2	H	175	THR
2	H	185	LEU
2	H	187	SER
2	H	192	SER
2	H	193	LEU
2	H	198	THR
2	H	216	LYS
2	H	230	SER
1	B	1	SER
1	B	12	LEU

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Mol	Chain	Res	Type
1	B	19	ARG
1	B	21	THR
1	B	30	VAL
1	B	51	SER
1	B	57	SER
1	B	68	SER
1	B	75	THR
1	B	78	SER
1	B	103	GLN
1	B	145	ARG
1	B	165	SER
1	B	179	SER
1	B	200	THR
2	A	4	GLU
2	A	15	VAL
2	A	16	GLN
2	A	20	SER
2	A	21	LEU
2	A	33	SER
2	A	53	TYR
2	A	62	SER
2	A	67	VAL
2	A	68	LYS
2	A	101	ARG
2	A	122	THR
2	A	153	LEU
2	A	155	CYS
2	A	156	LEU
2	A	157	VAL
2	A	158	LYS
2	A	165	VAL
2	A	175	THR
2	A	185	LEU
2	A	187	SER
2	A	192	SER
2	A	193	LEU
2	A	212	ASN
2	A	226	VAL
2	A	227	GLU
3	R	17	LYS
3	R	28	THR
3	R	39	THR

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Mol	Chain	Res	Type
3	R	56	THR
3	R	70	SER
3	R	73	ARG
3	R	74	THR
3	R	78	MET
3	R	80	ASN
3	R	84	GLN
3	R	85	MET
3	R	123	LEU
3	R	128	SER
3	R	132	LEU
3	R	133	ILE
3	R	140	PHE
3	R	141	THR
3	R	142	LEU
3	R	143	LEU
3	R	148	LEU
3	R	158	ILE
3	R	165	THR
3	R	170	LEU
3	R	171	SER
3	R	173	HIS
3	R	179	LEU
3	R	182	VAL
3	R	183	ARG
3	R	202	ILE
3	R	208	MET
3	R	210	ASP
3	R	211	THR
3	C	25	ARG
3	C	29	ASP
3	C	32	LEU
3	C	34	THR
3	C	38	LEU
3	C	42	ARG
3	C	47	LEU
3	C	56	THR
3	C	67	GLN
3	C	73	ARG
3	C	78	MET
3	C	80	ASN
3	C	82	THR

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Mol	Chain	Res	Type
3	C	88	SER
3	C	93	LEU
3	C	100	ILE
3	C	107	LEU
3	C	122	TYR
3	C	123	LEU
3	C	128	SER
3	C	131	THR
3	C	133	ILE
3	C	135	LEU
3	C	137	THR
3	C	139	TRP
3	C	140	PHE
3	C	143	LEU
3	C	148	LEU
3	C	151	GLU
3	C	164	GLN
3	C	168	LYS
3	C	169	ILE
3	C	170	LEU
3	C	179	LEU
3	C	180	VAL
3	C	182	VAL
3	C	183	ARG
3	C	184	CYS
3	C	201	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	4	GLN
1	L	103	GLN
1	L	201	HIS
1	L	202	GLN
1	L	213	ASN
2	H	16	GLN
2	H	38	HIS
2	H	207	GLN
1	B	103	GLN
1	B	201	HIS
2	A	16	GLN
2	A	38	HIS

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Mol	Chain	Res	Type
2	A	207	GLN
2	A	214	ASN
3	R	41	HIS
3	R	49	HIS
3	R	80	ASN
3	R	83	ASN
3	R	115	GLN
3	C	67	GLN
3	C	83	ASN
3	C	159	HIS
3	C	201	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](#)

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

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	$\# Z > 2$
4	GOL	C	301	-	5,5,5	0.52	0	5,5,5	0.51	0
4	GOL	L	301	-	5,5,5	0.40	0	5,5,5	0.30	0
4	GOL	H	302	-	5,5,5	1.23	0	5,5,5	1.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	ACT	R	301	-	3,3,3	1.36	0	3,3,3	0.75	0
4	GOL	A	301	-	5,5,5	0.35	0	5,5,5	0.78	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
4	GOL	C	301	-	-	2/4/4/4	-
4	GOL	L	301	-	-	2/4/4/4	-
4	GOL	A	301	-	-	0/4/4/4	-
4	GOL	H	302	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	L	301	GOL	C1-C2-C3-O3
4	L	301	GOL	O2-C2-C3-O3
4	C	301	GOL	O1-C1-C2-C3
4	C	301	GOL	O1-C1-C2-O2
4	H	302	GOL	C1-C2-C3-O3
4	H	302	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	302	GOL	2	0
6	R	301	ACT	2	0

5.7 Other polymers [i](#)

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	B	215/217 (99%)	0.42	5 (2%) 60 50	34, 76, 121, 134	0
1	L	216/217 (99%)	-0.04	0 100 100	35, 51, 70, 89	0
2	A	220/236 (93%)	-0.08	6 (2%) 54 42	28, 42, 94, 116	0
2	H	227/236 (96%)	-0.19	0 100 100	28, 42, 88, 105	0
3	C	188/211 (89%)	0.64	21 (11%) 5 4	37, 71, 119, 144	0
3	R	205/211 (97%)	0.13	11 (5%) 25 16	30, 53, 109, 159	0
All	All	1271/1328 (95%)	0.13	43 (3%) 45 33	28, 52, 108, 159	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	121	PRO	5.6
1	B	215	GLY	5.0
3	C	178	TYR	4.1
3	C	113	VAL	3.9
3	C	122	TYR	3.8
1	B	77	SER	3.7
3	C	31	GLY	3.6
3	R	84	GLN	3.6
3	C	32	LEU	3.5
3	C	33	PRO	3.4
3	C	123	LEU	3.3
3	R	85	MET	3.1
3	C	124	TRP	3.0
3	R	82	THR	2.7
3	C	148	LEU	2.6
3	C	114	LYS	2.6
3	C	137	THR	2.6
3	C	34	THR	2.6
1	B	157	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
3	C	200	ILE	2.5
3	C	112	GLU	2.5
1	B	209	THR	2.4
3	C	35	ASN	2.4
3	C	111	VAL	2.3
3	R	83	ASN	2.3
3	R	86	GLY	2.3
1	B	156	ALA	2.3
2	A	149	GLY	2.3
3	R	80	ASN	2.2
2	A	203	SER	2.2
3	R	3	PRO	2.2
2	A	227	GLU	2.2
3	C	169	ILE	2.2
3	C	30	GLY	2.2
3	C	151	GLU	2.1
3	R	88	SER	2.1
3	R	139	TRP	2.1
2	A	202	SER	2.1
3	R	137	THR	2.1
3	R	73	ARG	2.1
2	A	228	PRO	2.0
3	C	84	GLN	2.0
2	A	204	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
4	GOL	H	302	6/6	0.77	0.30	37,53,61,62	0
4	GOL	L	301	6/6	0.79	0.40	46,55,66,75	0
5	CA	B	301	1/1	0.80	0.15	53,53,53,53	0
4	GOL	C	301	6/6	0.92	0.28	46,53,56,59	0
6	ACT	R	301	4/4	0.95	0.22	43,47,50,51	0
4	GOL	A	301	6/6	0.98	0.15	32,34,37,39	0
5	CA	H	301	1/1	0.98	0.07	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.