



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:26 PM UTC

PDB ID : 9KEF / pdb_00009kef
Title : Crystal structure of RABV-G in complex with SOJB-Fab complex
Authors : Lu, G.; Yang, F.; Lin, S.
Deposited on : 2024-11-05
Resolution : 3.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

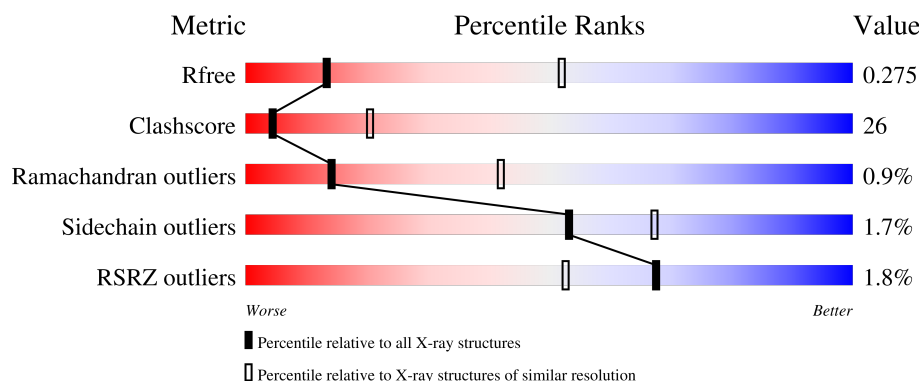
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	439	
2	H	239	
3	L	215	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6082 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 RABV-G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	0	0
			2833	1797	485	527	24			

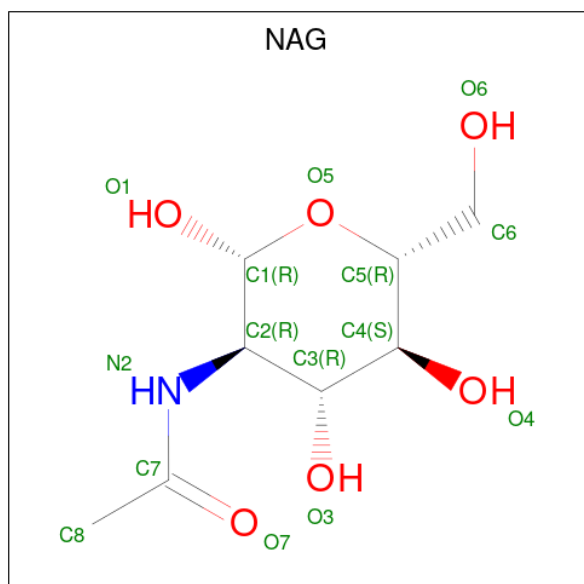
- Molecule 2 is a protein called SOJB-Fab Hchain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	214	Total	C	N	O	S	0	0	0
			1637	1043	271	317	6			

- Molecule 3 is a protein called SOJB-Fab Lchain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	210	Total	C	N	O	S	0	0	0
			1598	995	274	325	4			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

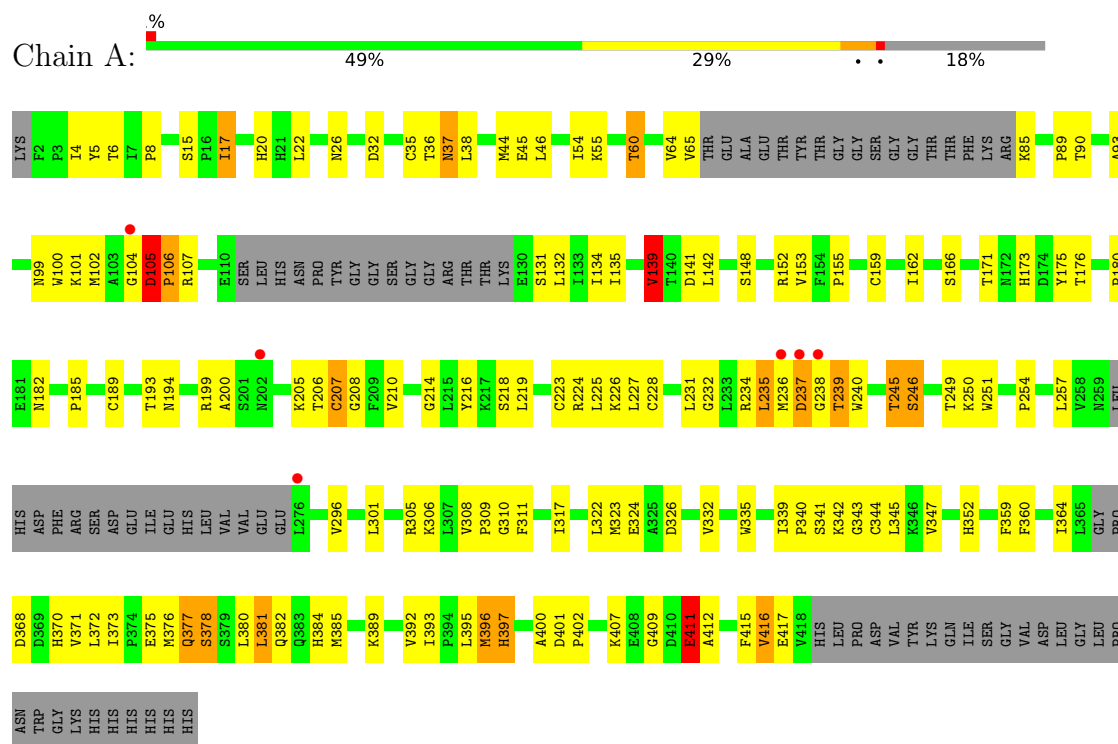


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

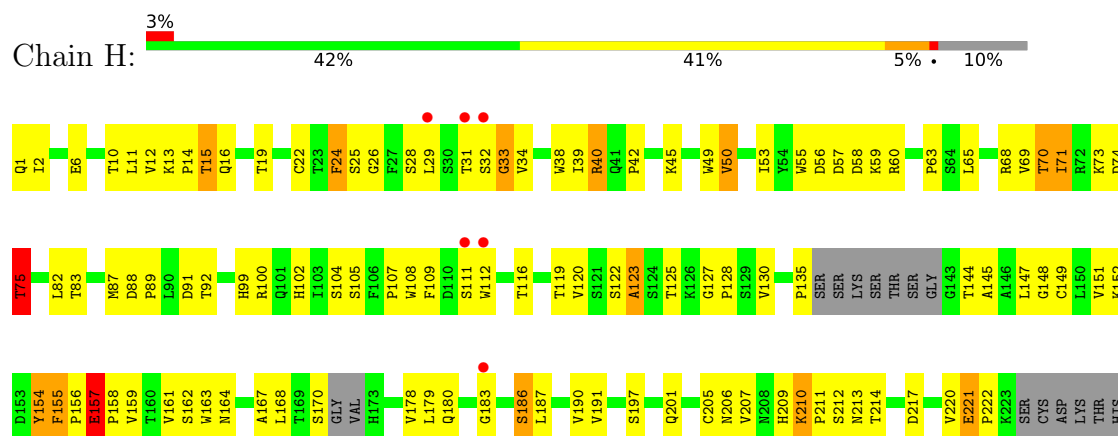
3 Residue-property plots

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: RABV-G

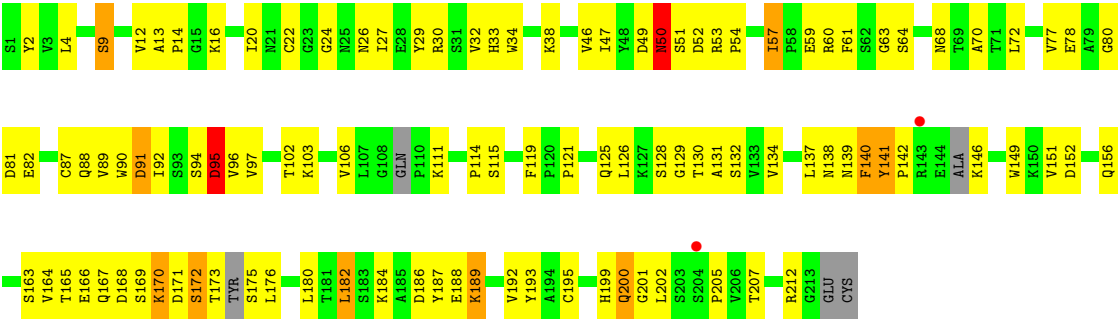


• Molecule 2: SOJB-Fab Hchain



THR
GLY
GLY
SER
HIS
HIS
HIS
HIS
HIS
HIS

● Molecule 3: SOJB-Fab Lchian



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	84.18Å 154.42Å 191.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.84 – 3.40 37.84 – 3.40	Depositor EDS
% Data completeness (in resolution range)	95.5 (37.84-3.40) 95.4 (37.84-3.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 3.40Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.217 , 0.264 0.240 , 0.275	Depositor DCC
R_{free} test set	894 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	89.8	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 86.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.010 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.030 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6082	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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

5.1 Standard geometry

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

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	0.58	0/2901	1.18	40/3929 (1.0%)
2	H	0.56	0/1680	1.23	30/2297 (1.3%)
3	L	0.54	0/1630	1.08	20/2211 (0.9%)
All	All	0.56	0/6211	1.17	90/8437 (1.1%)

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	H	0	1
3	L	0	1
All	All	0	2

There are no bond length outliers.

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	411	GLU	N-CA-C	-21.18	72.52	108.75
2	H	167	ALA	N-CA-C	-12.13	97.95	113.72
1	A	411	GLU	N-CA-CB	11.14	131.29	111.13
1	A	245	THR	CB-CA-C	-10.59	94.38	110.26
2	H	75	THR	N-CA-C	-10.53	97.82	113.61
1	A	309	PRO	CB-CA-C	-10.15	97.71	111.21
1	A	382	GLN	N-CA-C	-10.09	100.51	113.12
3	L	51	SER	N-CA-C	9.96	126.65	113.30
2	H	157	GLU	N-CA-C	-9.52	98.12	109.93
2	H	25	SER	N-CA-C	9.23	125.28	112.45
3	L	82	GLU	N-CA-C	-9.14	93.30	108.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	415	PHE	N-CA-C	-9.07	91.93	107.99
1	A	393	ILE	N-CA-C	-9.03	97.44	107.73
2	H	25	SER	N-CA-CB	-8.94	96.94	110.26
1	A	381	LEU	CB-CA-C	-8.87	94.22	110.63
3	L	95	ASP	N-CA-C	-8.62	99.63	112.04
2	H	74	ASP	N-CA-C	-8.50	93.19	108.48
2	H	24	PHE	CB-CA-C	-8.44	94.88	109.65
1	A	139	VAL	N-CA-C	-8.38	97.81	109.21
1	A	245	THR	N-CA-C	8.36	121.88	109.59
1	A	416	VAL	N-CA-C	-8.28	95.09	106.85
1	A	378	SER	N-CA-C	-8.26	103.20	113.28
2	H	144	THR	CB-CA-C	8.22	128.13	110.45
3	L	200	GLN	N-CA-C	8.07	120.08	111.28
1	A	246	SER	N-CA-CB	-8.03	97.15	110.47
2	H	116	THR	N-CA-C	7.76	121.44	110.50
2	H	24	PHE	N-CA-C	7.74	122.39	108.69
1	A	392	VAL	CB-CA-C	7.66	123.86	111.29
2	H	50	VAL	CB-CA-C	-7.54	103.52	110.91
3	L	200	GLN	CB-CA-C	-7.34	98.60	110.79
2	H	74	ASP	CB-CA-C	7.30	122.20	109.80
1	A	360	PHE	N-CA-C	7.26	119.69	110.33
2	H	75	THR	N-CA-CB	7.16	121.47	110.80
2	H	145	ALA	N-CA-C	-7.12	98.53	109.14
2	H	144	THR	N-CA-C	-7.02	98.39	109.07
2	H	154	TYR	CB-CA-C	6.98	121.44	109.51
3	L	189	LYS	N-CA-C	6.91	121.87	113.17
3	L	57	ILE	N-CA-C	6.91	114.57	108.63
2	H	220	VAL	N-CA-C	-6.88	97.58	107.77
3	L	169	SER	CB-CA-C	6.84	122.14	110.79
3	L	9	SER	N-CA-C	6.82	120.78	111.17
1	A	412	ALA	N-CA-C	-6.78	98.68	109.59
1	A	411	GLU	CB-CA-C	6.70	122.94	109.68
3	L	52	ASP	N-CA-C	6.60	120.63	110.20
1	A	310	GLY	N-CA-C	-6.58	101.03	110.38
1	A	60	THR	CB-CA-C	6.58	120.67	110.14
1	A	60	THR	N-CA-C	-6.55	97.59	108.34
1	A	106	PRO	N-CA-C	-6.47	107.22	114.92
2	H	50	VAL	N-CA-C	6.26	117.38	112.12
1	A	235	LEU	N-CA-C	6.18	122.56	110.56
1	A	36	THR	N-CA-CB	-6.18	101.27	110.61
2	H	40	ARG	CB-CA-C	-6.14	97.64	109.37
3	L	170	LYS	N-CA-CB	-6.10	100.63	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	50	ASN	N-CA-C	-6.08	97.86	110.80
2	H	221	GLU	N-CA-CB	6.06	119.79	111.25
1	A	236	MET	N-CA-CB	6.06	120.76	110.71
1	A	397	HIS	N-CA-C	-6.01	101.79	110.08
1	A	37	ASN	N-CA-C	-5.99	100.78	109.59
3	L	140	PHE	N-CA-C	5.96	119.30	110.48
2	H	186	SER	CB-CA-C	5.94	120.55	109.86
2	H	16	GLN	N-CA-C	-5.92	101.42	109.95
2	H	154	TYR	N-CA-C	-5.86	101.00	110.32
2	H	70	THR	CB-CA-C	5.84	118.77	110.24
1	A	396	MET	CB-CA-C	5.72	121.34	109.38
2	H	70	THR	N-CA-C	-5.71	98.30	108.13
2	H	220	VAL	CB-CA-C	5.67	118.07	110.42
2	H	123	ALA	N-CA-CB	5.60	120.90	110.99
1	A	239	THR	CB-CA-C	5.56	116.63	109.80
1	A	409	GLY	CA-C-O	-5.55	118.14	122.52
3	L	64	SER	CB-CA-C	-5.47	100.44	111.17
2	H	145	ALA	N-CA-CB	5.47	120.48	111.62
1	A	396	MET	CA-C-N	5.46	128.98	120.68
1	A	396	MET	C-N-CA	5.46	128.98	120.68
3	L	51	SER	N-CA-CB	-5.41	102.45	110.61
1	A	416	VAL	N-CA-CB	5.39	118.47	111.83
3	L	9	SER	CB-CA-C	-5.27	103.79	112.06
1	A	359	PHE	N-CA-C	-5.27	102.22	110.17
1	A	239	THR	N-CA-C	-5.26	102.85	110.64
1	A	377	GLN	N-CA-C	5.26	122.01	110.80
1	A	17	ILE	CB-CA-C	-5.24	102.29	110.52
1	A	214	GLY	N-CA-C	5.17	122.23	115.36
3	L	201	GLY	N-CA-C	-5.16	106.12	113.86
3	L	91	ASP	CB-CA-C	5.16	121.95	111.11
3	L	170	LYS	CB-CA-C	5.12	120.59	111.03
1	A	381	LEU	N-CA-C	5.11	117.58	111.71
3	L	182	LEU	N-CA-C	-5.10	102.61	109.95
2	H	71	ILE	N-CA-C	-5.05	101.38	109.20
2	H	15	THR	CB-CA-C	-5.04	101.84	111.06
1	A	309	PRO	N-CA-C	5.03	119.09	111.19
1	A	36	THR	N-CA-C	5.03	120.03	113.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	157	GLU	Peptide
3	L	141	TYR	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	A	2833	0	2782	127	1
2	H	1637	0	1621	109	0
3	L	1598	0	1543	103	1
4	A	14	0	13	0	0
All	All	6082	0	5959	318	1

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 26.

All (318) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:125:THR:HG23	2:H:156:PRO:HG2	1.24	1.13
1:A:245:THR:HG23	1:A:245:THR:O	1.61	0.99
2:H:14:PRO:O	2:H:15:THR:HG22	1.62	0.99
2:H:28:SER:HB2	2:H:31:THR:HG23	1.46	0.98
3:L:167:GLN:NE2	3:L:172:SER:O	1.99	0.95
1:A:90:THR:HG23	1:A:93:ALA:HB3	1.50	0.94
3:L:121:PRO:HB3	3:L:132:SER:H	1.37	0.90
1:A:377:GLN:O	1:A:381:LEU:HG	1.73	0.87
2:H:24:PHE:O	2:H:24:PHE:CD1	2.30	0.84
2:H:10:THR:HG23	2:H:11:LEU:HD12	1.60	0.83
3:L:166:GLU:HG3	3:L:167:GLN:H	1.44	0.82
2:H:155:PHE:HB3	2:H:156:PRO:HD3	1.62	0.81
2:H:161:VAL:HG22	2:H:207:VAL:HG22	1.64	0.79
1:A:228:CYS:HA	2:H:60:ARG:HH22	1.47	0.79
1:A:341:SER:HB3	1:A:344:CYS:HB3	1.65	0.76
2:H:89:PRO:HA	2:H:120:VAL:HG13	1.66	0.75
2:H:68:ARG:NH2	2:H:91:ASP:OD2	2.19	0.75
1:A:199:ARG:NH1	1:A:206:THR:HG21	2.02	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:GLN:O	1:A:381:LEU:CD2	2.36	0.73
1:A:64:VAL:HG23	1:A:131:SER:HB2	1.69	0.73
2:H:92:THR:HG23	2:H:119:THR:HA	1.70	0.72
1:A:100:TRP:CD2	1:A:106:PRO:HG2	2.25	0.71
1:A:401:ASP:OD1	1:A:402:PRO:HD2	1.91	0.70
1:A:44:MET:HE1	3:L:90:TRP:HZ3	1.57	0.70
1:A:245:THR:O	1:A:245:THR:CG2	2.36	0.70
1:A:381:LEU:O	1:A:385:MET:HG2	1.91	0.70
3:L:54:PRO:HB2	3:L:57:ILE:HD13	1.74	0.70
1:A:234:ARG:HG3	1:A:238:GLY:HA2	1.74	0.69
2:H:34:VAL:HG12	2:H:102:HIS:HB3	1.75	0.68
2:H:40:ARG:O	2:H:40:ARG:HG3	1.91	0.68
2:H:162:SER:HB3	2:H:206:ASN:HB2	1.77	0.67
2:H:125:THR:HG23	2:H:156:PRO:CG	2.13	0.66
3:L:125:GLN:HG2	3:L:130:THR:O	1.94	0.66
3:L:90:TRP:HA	3:L:95:ASP:O	1.95	0.66
2:H:42:PRO:HG2	2:H:45:LYS:HB2	1.77	0.66
3:L:121:PRO:HG3	3:L:131:ALA:HB1	1.77	0.65
2:H:156:PRO:HD2	2:H:209:HIS:NE2	2.11	0.65
1:A:224:ARG:HE	1:A:231:LEU:HB3	1.61	0.65
1:A:153:VAL:HG12	1:A:171:THR:HB	1.79	0.65
1:A:254:PRO:HA	1:A:257:LEU:HD22	1.79	0.65
1:A:199:ARG:HH11	1:A:206:THR:HG21	1.61	0.64
2:H:179:LEU:HD13	2:H:180:GLN:O	1.97	0.64
3:L:140:PHE:CZ	3:L:175:SER:HB2	2.32	0.64
2:H:128:PRO:HD3	2:H:209:HIS:CB	2.29	0.63
3:L:188:GLU:O	3:L:212:ARG:NH2	2.32	0.63
2:H:99:HIS:HB3	2:H:111:SER:HB2	1.80	0.62
3:L:142:PRO:HD2	3:L:199:HIS:CE1	2.34	0.62
1:A:105:ASP:OD1	1:A:105:ASP:N	2.33	0.62
3:L:137:LEU:O	3:L:175:SER:N	2.33	0.62
1:A:231:LEU:HB2	2:H:105:SER:HA	1.81	0.62
2:H:63:PRO:HD3	3:L:94:SER:HB2	1.80	0.62
1:A:99:ASN:O	1:A:102:MET:HB2	1.99	0.61
2:H:100:ARG:NH2	2:H:104:SER:O	2.32	0.61
2:H:15:THR:HG23	2:H:15:THR:O	2.01	0.61
1:A:194:ASN:HB3	3:L:29:TYR:CD2	2.36	0.61
3:L:47:ILE:HD12	3:L:50:ASN:O	2.01	0.61
2:H:155:PHE:CB	2:H:156:PRO:HD3	2.31	0.60
3:L:16:LYS:O	3:L:77:VAL:HG23	2.00	0.60
2:H:123:ALA:HB3	2:H:155:PHE:CD1	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:195:CYS:O	3:L:207:THR:HA	2.01	0.60
1:A:364:ILE:HG13	1:A:372:LEU:HD21	1.83	0.60
3:L:47:ILE:CD1	3:L:63:GLY:HA3	2.31	0.60
1:A:235:LEU:HB2	1:A:239:THR:HB	1.83	0.60
1:A:35:CYS:O	1:A:200:ALA:HB1	2.00	0.59
2:H:210:LYS:N	2:H:211:PRO:HD2	2.17	0.59
1:A:17:ILE:O	1:A:322:LEU:HB3	2.02	0.59
1:A:372:LEU:H	1:A:372:LEU:HD23	1.68	0.59
2:H:157:GLU:CD	2:H:157:GLU:H	2.10	0.59
1:A:90:THR:CG2	1:A:93:ALA:HB3	2.28	0.58
2:H:127:GLY:HA2	2:H:209:HIS:CD2	2.38	0.58
1:A:182:ASN:HD22	1:A:185:PRO:HA	1.68	0.58
1:A:226:LYS:NZ	2:H:58:ASP:OD2	2.36	0.58
2:H:152:LYS:HA	2:H:186:SER:HB2	1.85	0.58
1:A:377:GLN:O	1:A:381:LEU:HD23	2.04	0.58
2:H:55:TRP:O	2:H:73:LYS:NZ	2.36	0.58
3:L:151:VAL:HB	3:L:156:GLN:NE2	2.18	0.58
2:H:154:TYR:HE1	2:H:157:GLU:HA	1.69	0.58
2:H:156:PRO:HB2	2:H:211:PRO:CG	2.34	0.58
3:L:114:PRO:HB3	3:L:140:PHE:HD2	1.70	0.57
3:L:2:TYR:HD2	3:L:97:VAL:HG21	1.68	0.57
3:L:34:TRP:CD1	3:L:47:ILE:HD11	2.40	0.57
2:H:128:PRO:HD3	2:H:209:HIS:HB2	1.86	0.57
3:L:49:ASP:O	3:L:50:ASN:HB2	2.04	0.57
3:L:186:ASP:HA	3:L:189:LYS:HG2	1.87	0.56
1:A:208:GLY:HA2	1:A:219:LEU:HD22	1.87	0.56
1:A:238:GLY:O	1:A:239:THR:C	2.48	0.56
1:A:107:ARG:HH11	1:A:107:ARG:HG3	1.71	0.56
1:A:227:LEU:HD22	1:A:240:TRP:CE2	2.41	0.56
3:L:121:PRO:HB3	3:L:132:SER:N	2.16	0.56
1:A:37:ASN:O	1:A:200:ALA:HA	2.06	0.56
1:A:45:GLU:HB3	1:A:193:THR:HG22	1.87	0.56
2:H:32:SER:HA	2:H:55:TRP:CD1	2.41	0.56
3:L:168:ASP:HB2	3:L:171:ASP:OD1	2.05	0.55
3:L:30:ARG:NH2	3:L:91:ASP:OD1	2.29	0.55
1:A:381:LEU:O	1:A:385:MET:CG	2.55	0.55
3:L:38:LYS:HE2	3:L:80:GLY:O	2.06	0.55
2:H:29:LEU:HD21	2:H:73:LYS:HG3	1.89	0.55
2:H:128:PRO:HB3	2:H:154:TYR:HB3	1.88	0.55
1:A:173:HIS:HE1	1:A:175:TYR:HB2	1.72	0.55
3:L:152:ASP:HA	3:L:192:VAL:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:108:TRP:HB3	3:L:33:HIS:CD2	2.41	0.54
2:H:179:LEU:HD21	2:H:183:GLY:HA2	1.90	0.54
3:L:53:ARG:HD3	3:L:61:PHE:O	2.06	0.54
1:A:104:GLY:HA2	1:A:107:ARG:HB3	1.88	0.54
1:A:199:ARG:HH22	1:A:245:THR:CG2	2.21	0.54
2:H:28:SER:CB	2:H:31:THR:HG23	2.28	0.54
3:L:60:ARG:NH2	3:L:81:ASP:OD2	2.37	0.54
1:A:38:LEU:HA	1:A:199:ARG:O	2.07	0.54
1:A:347:VAL:CG1	1:A:352:HIS:HB2	2.38	0.54
2:H:197:SER:HB2	2:H:201:GLN:HB3	1.89	0.54
1:A:44:MET:HE1	3:L:90:TRP:CZ3	2.42	0.54
3:L:9:SER:HA	3:L:103:LYS:O	2.08	0.54
1:A:208:GLY:HA3	1:A:216:TYR:OH	2.08	0.54
2:H:31:THR:O	2:H:55:TRP:CB	2.56	0.54
1:A:395:LEU:HD22	1:A:396:MET:H	1.72	0.53
1:A:162:ILE:HG13	1:A:166:SER:O	2.08	0.53
3:L:53:ARG:CZ	3:L:59:GLU:HA	2.38	0.53
2:H:156:PRO:HB2	2:H:211:PRO:HG3	1.89	0.53
1:A:306:LYS:HD3	1:A:308:VAL:O	2.08	0.53
1:A:107:ARG:NH2	1:A:134:ILE:H	2.07	0.53
3:L:140:PHE:CZ	3:L:176:LEU:HD23	2.44	0.53
1:A:208:GLY:HA3	1:A:216:TYR:CZ	2.44	0.53
1:A:377:GLN:O	1:A:381:LEU:CG	2.52	0.53
3:L:182:LEU:HB3	3:L:186:ASP:HB2	1.91	0.53
1:A:20:HIS:HB2	1:A:152:ARG:NH2	2.23	0.52
2:H:209:HIS:CE1	2:H:211:PRO:HG2	2.44	0.52
3:L:114:PRO:HB3	3:L:140:PHE:HB3	1.91	0.52
2:H:24:PHE:O	2:H:24:PHE:HD1	1.86	0.52
2:H:33:GLY:HA2	2:H:55:TRP:CZ3	2.45	0.52
2:H:130:VAL:HG22	2:H:151:VAL:HG13	1.92	0.52
3:L:20:ILE:HG12	3:L:102:THR:HG21	1.92	0.52
3:L:139:ASN:C	3:L:173:THR:HB	2.34	0.52
1:A:224:ARG:HG2	1:A:249:THR:HG23	1.91	0.52
2:H:29:LEU:HB3	2:H:75:THR:HB	1.91	0.52
1:A:199:ARG:HH22	1:A:245:THR:HG21	1.74	0.52
3:L:14:PRO:HG3	3:L:106:VAL:HG12	1.91	0.52
3:L:114:PRO:HB3	3:L:140:PHE:CD2	2.45	0.52
3:L:141:TYR:HA	3:L:142:PRO:O	2.09	0.52
1:A:205:LYS:HE2	1:A:206:THR:O	2.10	0.52
1:A:180:PRO:HG2	1:A:182:ASN:O	2.09	0.52
1:A:194:ASN:HB3	3:L:29:TYR:CE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:TYR:HE1	1:A:218:SER:HB2	1.73	0.52
1:A:225:LEU:HD22	1:A:227:LEU:CD1	2.40	0.52
1:A:335:TRP:CZ3	1:A:376:MET:HB2	2.45	0.52
2:H:49:TRP:CG	3:L:96:VAL:HG13	2.45	0.52
3:L:12:VAL:HG21	3:L:77:VAL:HG21	1.91	0.52
3:L:34:TRP:CZ3	3:L:72:LEU:HD22	2.44	0.52
3:L:187:TYR:HA	3:L:193:TYR:OH	2.08	0.52
1:A:60:THR:O	1:A:134:ILE:HA	2.10	0.51
1:A:207:CYS:C	1:A:219:LEU:HD23	2.35	0.51
1:A:342:LYS:HD2	1:A:370:HIS:CE1	2.44	0.51
2:H:148:GLY:HA3	2:H:190:VAL:HG12	1.93	0.51
3:L:171:ASP:O	3:L:172:SER:HB2	2.10	0.51
1:A:235:LEU:N	1:A:239:THR:O	2.30	0.51
2:H:2:ILE:HA	2:H:26:GLY:HA3	1.92	0.51
1:A:347:VAL:HG12	1:A:352:HIS:HB2	1.93	0.51
3:L:129:GLY:HA2	3:L:184:LYS:HB2	1.92	0.51
2:H:13:LYS:HE2	2:H:122:SER:OG	2.12	0.50
3:L:34:TRP:CZ3	3:L:87:CYS:HB3	2.46	0.50
1:A:381:LEU:O	1:A:385:MET:HB2	2.10	0.50
3:L:77:VAL:HG12	3:L:78:GLU:O	2.12	0.50
3:L:164:VAL:HG22	3:L:176:LEU:HB2	1.93	0.50
1:A:373:ILE:HB	1:A:376:MET:HB3	1.94	0.50
2:H:82:LEU:HD12	2:H:83:THR:N	2.26	0.50
3:L:4:LEU:H	3:L:4:LEU:HD23	1.77	0.50
2:H:12:VAL:O	2:H:120:VAL:HA	2.11	0.50
2:H:69:VAL:HG23	2:H:82:LEU:CD1	2.42	0.49
3:L:34:TRP:HB2	3:L:47:ILE:HG12	1.93	0.49
1:A:5:TYR:HE1	1:A:375:GLU:OE1	1.95	0.49
1:A:17:ILE:HG21	1:A:324:GLU:CD	2.37	0.49
2:H:109:PHE:HB2	2:H:112:TRP:CZ2	2.47	0.49
1:A:343:GLY:HA2	1:A:371:VAL:HG23	1.95	0.49
2:H:135:PRO:HD3	2:H:147:LEU:HB3	1.95	0.49
2:H:163:TRP:CH2	2:H:205:CYS:HB3	2.48	0.49
3:L:111:LYS:HD2	3:L:200:GLN:HB3	1.95	0.49
2:H:65:LEU:O	2:H:69:VAL:HG12	2.13	0.48
2:H:31:THR:O	2:H:55:TRP:CG	2.66	0.48
3:L:26:ASN:H	3:L:68:ASN:ND2	2.11	0.48
2:H:6:GLU:CD	2:H:6:GLU:H	2.19	0.48
3:L:47:ILE:HD13	3:L:63:GLY:HA3	1.96	0.48
2:H:40:ARG:O	2:H:40:ARG:CG	2.61	0.48
1:A:54:ILE:HB	1:A:142:LEU:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:53:ILE:HB	2:H:71:ILE:HD13	1.96	0.48
2:H:29:LEU:CD2	2:H:73:LYS:HG3	2.44	0.48
1:A:296:VAL:HG21	1:A:301:LEU:HD13	1.95	0.48
2:H:63:PRO:CD	3:L:94:SER:HB2	2.42	0.48
3:L:138:ASN:HA	3:L:175:SER:N	2.29	0.48
3:L:129:GLY:O	3:L:184:LYS:N	2.44	0.48
3:L:141:TYR:HA	3:L:142:PRO:C	2.39	0.48
2:H:107:PRO:HD2	3:L:90:TRP:HB2	1.96	0.47
1:A:4:ILE:HG12	1:A:332:VAL:O	2.13	0.47
1:A:8:PRO:O	1:A:347:VAL:HG23	2.14	0.47
2:H:50:VAL:HG13	2:H:65:LEU:HD13	1.96	0.47
1:A:107:ARG:HH21	1:A:134:ILE:H	1.63	0.47
2:H:68:ARG:HH22	2:H:91:ASP:CG	2.20	0.47
2:H:70:THR:N	2:H:83:THR:O	2.48	0.47
3:L:46:VAL:HA	3:L:57:ILE:HG12	1.96	0.47
2:H:53:ILE:HD13	2:H:73:LYS:HB2	1.96	0.47
2:H:125:THR:CG2	2:H:156:PRO:HG2	2.17	0.47
2:H:206:ASN:HA	2:H:217:ASP:OD1	2.14	0.47
2:H:157:GLU:OE1	2:H:157:GLU:N	2.41	0.47
3:L:12:VAL:HG22	3:L:13:ALA:N	2.29	0.47
1:A:162:ILE:HD13	1:A:180:PRO:HG3	1.96	0.47
2:H:56:ASP:O	2:H:57:ASP:C	2.58	0.47
3:L:164:VAL:HG12	3:L:165:THR:O	2.14	0.47
1:A:6:THR:OG1	1:A:305:ARG:NH1	2.48	0.47
1:A:65:VAL:O	1:A:85:LYS:HE3	2.14	0.47
1:A:100:TRP:O	1:A:104:GLY:N	2.41	0.47
2:H:39:ILE:N	2:H:39:ILE:HD12	2.30	0.46
3:L:49:ASP:O	3:L:50:ASN:CB	2.63	0.46
1:A:173:HIS:CE1	1:A:175:TYR:HD2	2.33	0.46
1:A:231:LEU:HD22	2:H:100:ARG:NH2	2.31	0.46
3:L:149:TRP:CG	3:L:180:LEU:HD13	2.50	0.46
1:A:6:THR:OG1	1:A:306:LYS:O	2.33	0.46
1:A:26:ASN:HB3	1:A:237:ASP:OD1	2.16	0.46
1:A:105:ASP:CG	1:A:106:PRO:HD3	2.41	0.46
2:H:159:VAL:HB	2:H:187:LEU:HD21	1.98	0.46
3:L:34:TRP:CH2	3:L:72:LEU:HD22	2.51	0.46
2:H:60:ARG:HG3	3:L:95:ASP:OD2	2.16	0.46
1:A:207:CYS:O	1:A:219:LEU:HD23	2.16	0.45
3:L:188:GLU:O	3:L:212:ARG:CZ	2.64	0.45
1:A:345:LEU:HD12	1:A:345:LEU:HA	1.77	0.45
2:H:38:TRP:CG	2:H:82:LEU:HD22	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:87:MET:HE3	2:H:87:MET:HB3	1.86	0.45
3:L:115:SER:O	3:L:137:LEU:HA	2.17	0.45
2:H:22:CYS:HB2	2:H:38:TRP:CZ2	2.51	0.45
3:L:32:VAL:HA	3:L:89:VAL:HG12	1.98	0.45
1:A:22:LEU:HD21	1:A:322:LEU:HD21	1.99	0.45
2:H:14:PRO:O	2:H:15:THR:CG2	2.50	0.45
3:L:142:PRO:HG2	3:L:200:GLN:OE1	2.16	0.45
1:A:326:ASP:OD1	1:A:326:ASP:N	2.48	0.45
1:A:173:HIS:HB3	1:A:176:THR:HB	1.98	0.45
2:H:14:PRO:CG	2:H:122:SER:HB2	2.47	0.45
2:H:31:THR:O	2:H:55:TRP:HB2	2.16	0.45
2:H:178:VAL:HG23	3:L:163:SER:HB2	1.98	0.45
1:A:134:ILE:C	1:A:135:ILE:HG13	2.42	0.45
1:A:417:GLU:O	1:A:417:GLU:HG2	2.17	0.45
2:H:60:ARG:HD3	2:H:60:ARG:HA	1.58	0.44
2:H:221:GLU:HB2	2:H:222:PRO:HD2	2.00	0.44
3:L:142:PRO:HD2	3:L:199:HIS:NE2	2.32	0.44
3:L:125:GLN:O	3:L:128:SER:OG	2.34	0.44
1:A:407:LYS:HB2	1:A:411:GLU:OE2	2.18	0.44
1:A:55:LYS:HD3	1:A:141:ASP:OD1	2.18	0.44
3:L:187:TYR:O	3:L:212:ARG:HD3	2.17	0.44
1:A:148:SER:HB2	1:A:159:CYS:O	2.18	0.43
1:A:339:ILE:HD12	1:A:376:MET:HE1	1.99	0.43
3:L:199:HIS:O	3:L:202:LEU:HB2	2.18	0.43
1:A:250:LYS:HE3	1:A:250:LYS:HB2	1.85	0.43
2:H:69:VAL:HG23	2:H:82:LEU:HD11	2.00	0.43
3:L:88:GLN:CG	3:L:96:VAL:HG23	2.49	0.43
3:L:91:ASP:CG	3:L:92:ILE:H	2.27	0.43
1:A:210:VAL:O	1:A:210:VAL:HG23	2.17	0.43
1:A:376:MET:O	1:A:380:LEU:HD22	2.18	0.43
2:H:210:LYS:N	2:H:211:PRO:CD	2.81	0.43
1:A:395:LEU:HD13	1:A:396:MET:C	2.43	0.43
2:H:28:SER:HB2	2:H:31:THR:CG2	2.32	0.43
2:H:210:LYS:O	2:H:211:PRO:C	2.62	0.43
3:L:22:CYS:HB2	3:L:34:TRP:CH2	2.53	0.43
3:L:4:LEU:HD13	3:L:89:VAL:HG22	2.00	0.43
3:L:20:ILE:HB	3:L:72:LEU:CD2	2.49	0.43
3:L:24:GLY:N	3:L:27:ILE:HD12	2.33	0.43
1:A:237:ASP:HB3	1:A:311:PHE:HB3	2.00	0.43
3:L:22:CYS:O	3:L:70:ALA:N	2.52	0.43
3:L:91:ASP:CG	3:L:92:ILE:N	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LEU:HD12	1:A:234:ARG:HB2	2.00	0.42
3:L:121:PRO:CG	3:L:131:ALA:HB1	2.48	0.42
3:L:170:LYS:HE3	3:L:170:LYS:HB2	1.91	0.42
1:A:223:CYS:HB2	1:A:251:TRP:C	2.44	0.42
3:L:34:TRP:HD1	3:L:47:ILE:HD11	1.83	0.42
1:A:225:LEU:HD22	1:A:227:LEU:HD13	2.01	0.42
2:H:170:SER:O	2:H:191:VAL:HG23	2.19	0.42
1:A:46:LEU:HD23	1:A:46:LEU:HA	1.74	0.42
1:A:228:CYS:CA	2:H:60:ARG:HH22	2.25	0.42
2:H:49:TRP:CG	3:L:96:VAL:CG1	3.03	0.42
1:A:208:GLY:HA2	1:A:219:LEU:CD2	2.50	0.42
1:A:246:SER:CB	2:H:104:SER:HA	2.49	0.42
3:L:146:LYS:HA	3:L:146:LYS:HD2	1.74	0.42
1:A:55:LYS:HD2	1:A:139:VAL:HG13	2.01	0.42
2:H:212:SER:O	2:H:213:ASN:C	2.62	0.42
3:L:72:LEU:HD23	3:L:72:LEU:H	1.85	0.42
1:A:100:TRP:CE3	1:A:106:PRO:HG2	2.55	0.42
1:A:397:HIS:HB3	1:A:400:ALA:HB2	2.02	0.42
3:L:90:TRP:CE2	3:L:91:ASP:O	2.72	0.42
1:A:15:SER:C	1:A:323:MET:HE2	2.45	0.41
2:H:19:THR:HA	2:H:82:LEU:O	2.19	0.41
1:A:155:PRO:HD3	1:A:171:THR:HA	2.02	0.41
2:H:59:LYS:HB3	2:H:71:ILE:CG2	2.50	0.41
1:A:89:PRO:HB3	1:A:132:LEU:HD22	2.02	0.41
1:A:232:GLY:HA3	1:A:240:TRP:CZ2	2.56	0.41
3:L:16:LYS:HD2	3:L:16:LYS:HA	1.82	0.41
1:A:101:LYS:HE2	1:A:134:ILE:O	2.20	0.41
1:A:381:LEU:O	1:A:385:MET:CB	2.69	0.41
2:H:164:ASN:ND2	2:H:168:LEU:HD22	2.34	0.41
1:A:45:GLU:HB3	1:A:193:THR:CG2	2.50	0.41
1:A:395:LEU:HD22	1:A:396:MET:N	2.35	0.41
3:L:91:ASP:O	3:L:94:SER:O	2.38	0.41
1:A:194:ASN:HB3	3:L:29:TYR:CG	2.55	0.41
1:A:322:LEU:HD12	1:A:322:LEU:HA	1.77	0.41
2:H:24:PHE:O	2:H:24:PHE:CG	2.70	0.41
2:H:162:SER:O	2:H:206:ASN:N	2.36	0.41
2:H:212:SER:C	2:H:214:THR:N	2.77	0.41
3:L:166:GLU:HG3	3:L:167:GLN:N	2.23	0.41
1:A:368:ASP:OD2	1:A:370:HIS:HB2	2.21	0.41
1:A:384:HIS:O	1:A:385:MET:C	2.64	0.41
1:A:32:ASP:OD2	1:A:216:TYR:OH	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:SER:HB3	2:H:104:SER:HA	2.03	0.40
2:H:1:GLN:OE1	2:H:1:GLN:HA	2.21	0.40
2:H:88:ASP:O	2:H:120:VAL:HG11	2.21	0.40
3:L:119:PHE:HB2	3:L:134:VAL:HB	2.03	0.40
1:A:55:LYS:HD2	1:A:139:VAL:CG1	2.51	0.40
3:L:171:ASP:O	3:L:172:SER:CB	2.69	0.40
1:A:317:ILE:HB	1:A:322:LEU:HD12	2.04	0.40
1:A:389:LYS:HA	1:A:389:LYS:HD3	1.82	0.40
2:H:60:ARG:NH1	3:L:95:ASP:OD1	2.54	0.40
3:L:12:VAL:HG22	3:L:13:ALA:H	1.86	0.40
2:H:34:VAL:HG12	2:H:102:HIS:CB	2.46	0.40
2:H:210:LYS:H	2:H:210:LYS:NZ	2.19	0.40
3:L:126:LEU:O	3:L:184:LYS:HE3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ASN:OD1	3:L:205:PRO:CD[3_554]	2.05	0.15

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	351/439 (80%)	327 (93%)	22 (6%)	2 (1%)	21	50
2	H	208/239 (87%)	197 (95%)	8 (4%)	3 (1%)	9	31
3	L	202/215 (94%)	188 (93%)	12 (6%)	2 (1%)	12	40
All	All	761/893 (85%)	712 (94%)	42 (6%)	7 (1%)	14	42

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	50	ASN
2	H	155	PHE
3	L	172	SER
2	H	158	PRO
2	H	33	GLY
1	A	105	ASP
1	A	340	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	321/387 (83%)	313 (98%)	8 (2%)	42	62
2	H	190/211 (90%)	187 (98%)	3 (2%)	55	68
3	L	181/185 (98%)	180 (99%)	1 (1%)	78	80
All	All	692/783 (88%)	680 (98%)	12 (2%)	53	67

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ASP
1	A	139	VAL
1	A	189	CYS
1	A	207	CYS
1	A	237	ASP
1	A	378	SER
1	A	411	GLU
1	A	416	VAL
2	H	75	THR
2	H	149	CYS
2	H	210	LYS
3	L	95	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	57	ASN
1	A	182	ASN
1	A	194	ASN
1	A	352	HIS
2	H	180	GLN
2	H	209	HIS
3	L	125	GLN

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 ⓘ

1 ligand is 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	$\# Z > 2$
4	NAG	A	501	1	14,14,15	1.04	1 (7%)	17,19,21	0.53	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	NAG	A	501	1	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	501	NAG	C1-C2	3.27	1.56	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	NAG	C4-C5-C6-O6
4	A	501	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	361/439 (82%)	0.05	6 (1%)	69 54	58, 89, 119, 136	0
2	H	214/239 (89%)	0.08	6 (2%)	55 41	55, 84, 135, 154	0
3	L	210/215 (97%)	0.16	2 (0%)	79 66	61, 99, 160, 170	0
All	All	785/893 (87%)	0.09	14 (1%)	67 53	55, 90, 152, 170	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	237	ASP	6.6
2	H	32	SER	4.1
2	H	29	LEU	3.5
2	H	111	SER	3.2
1	A	236	MET	3.2
1	A	202	ASN	3.2
1	A	238	GLY	3.1
2	H	112	TRP	2.7
2	H	31	THR	2.7
2	H	183	GLY	2.6
3	L	204	SER	2.5
3	L	143	ARG	2.2
1	A	104	GLY	2.1
1	A	276	LEU	2.1

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

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
4	NAG	A	501	14/15	0.56	0.10	117,141,143,144	0

6.5 Other polymers [i](#)

There are no such residues in this entry.