



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:36 PM GMT

PDB ID : 2HPY
Title : Crystallographic model of lumirhodopsin
Authors : Nakamichi, H.; Okada, T.
Deposited on : 2006-07-18
Resolution : 2.80 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>

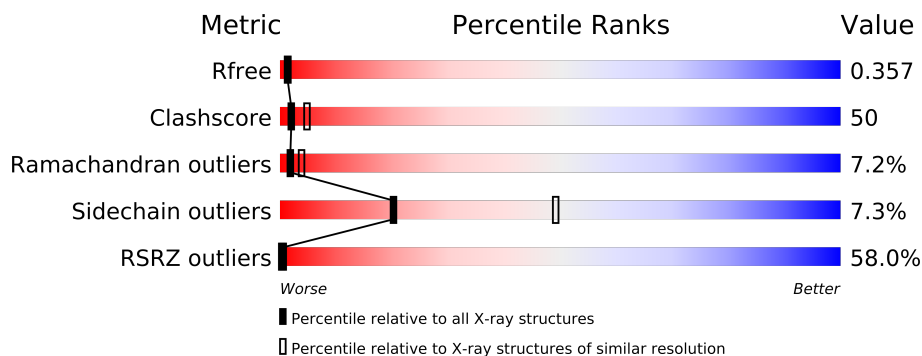
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.80 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	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

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	349	
1	B	349	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
7	RET	A	1296	-	X
7	RET	B	1296	-	X
8	PLM	A	1322	-	X
8	PLM	B	1407	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 5948 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 Rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2749	1818	424	481	26			
1	B	349	Total	C	N	O	S	0	0	0
			2749	1818	424	481	26			

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 3 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

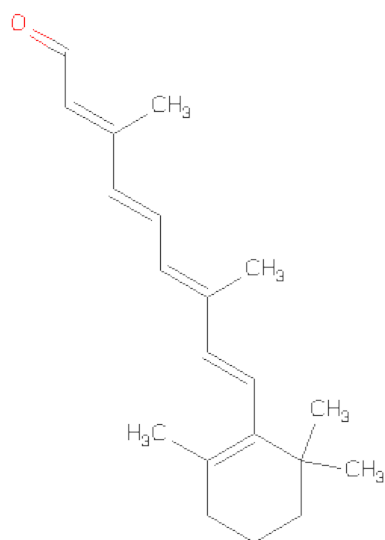
- Molecule 5 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	3	Total	Hg	0	0
			3	3		
5	A	3	Total	Hg	0	0
			3	3		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	3	Total	Zn	0	0
			3	3		
6	A	4	Total	Zn	0	0
			4	4		

- Molecule 7 is RETINAL (three-letter code: RET) (formula: C₂₀H₂₈O).



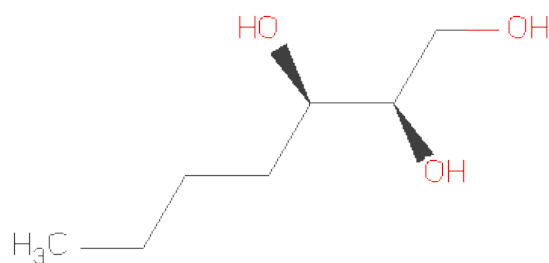
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	C	0	0
			20	20		
7	B	1	Total	C	0	0
			20	20		

- Molecule 8 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



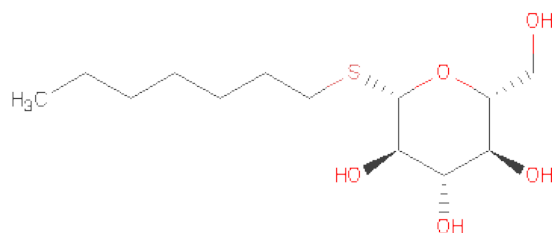
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			17	16	1		
8	A	1	Total	C	O	0	0
			17	16	1		
8	B	1	Total	C	O	0	0
			17	16	1		
8	B	1	Total	C	O	0	0
			17	16	1		
8	B	1	Total	C		0	0
			16	16			
8	A	1	Total	C		0	0
			16	16			

- Molecule 9 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: C₇H₁₆O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			10	7	3		

- Molecule 10 is HEPTYL 1-THIOHEXOPYRANOSIDE (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	O	S	0	0
			19	13	5	1		
10	A	1	Total	C	O	S	0	0
			19	13	5	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	O	S	0	0
			19	13	5	1		
10	B	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 11 is water.

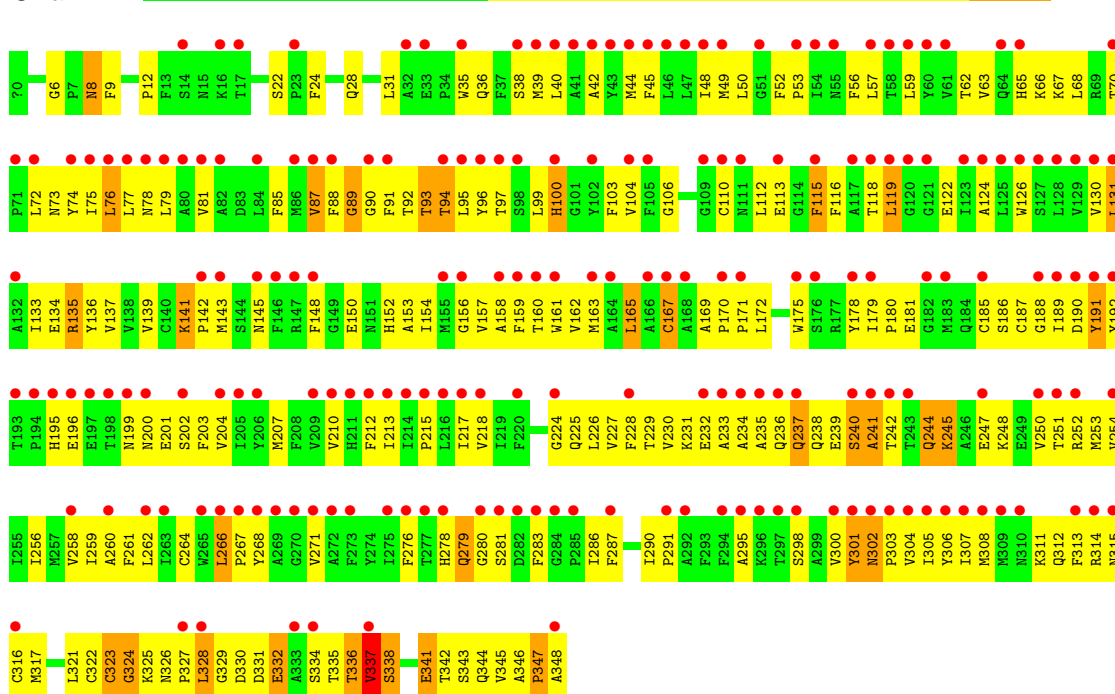
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	37	Total	O	0	0
			37	37		
11	B	29	Total	O	0	0
			29	29		

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.

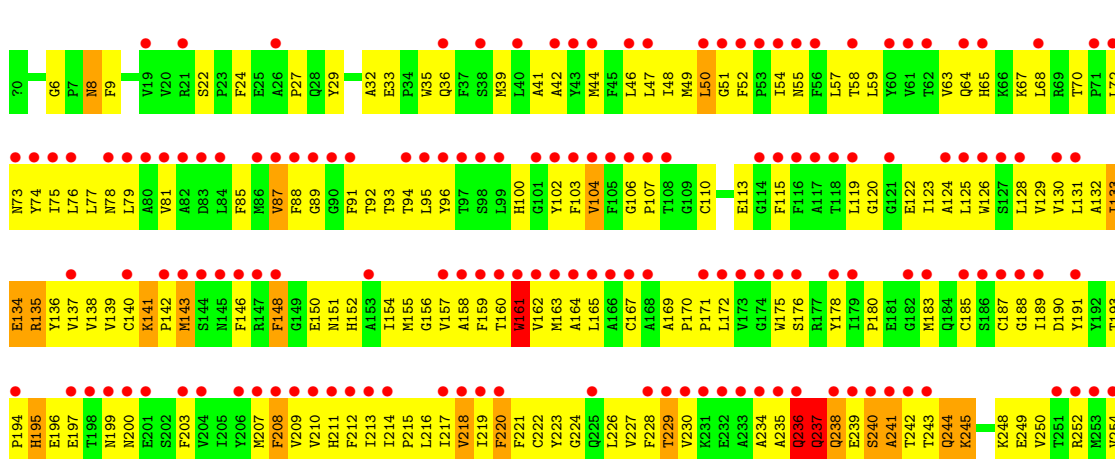
• Molecule 1: Rhodopsin

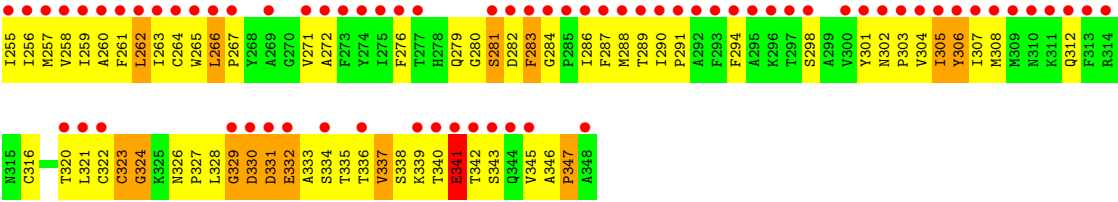
Chain A:



• Molecule 1: Rhodopsin

Chain B:





4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	96.72Å 96.72Å 150.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 35.05 – 2.79	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.80) 87.3 (35.05-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.218 , 0.238 0.355 , 0.357	Depositor DCC
R_{free} test set	1531 reflections (5.41%)	DCC
Wilson B-factor (Å ²)	64.8	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 103.5	EDS
Estimated twinning fraction	0.138 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 29870 reflections	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	5948	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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: HTG, ZN, BMA, NAG, ACE, HTO, RET, PLM, HG, MAN

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	0.65	0/2831	0.70	0/3859
1	B	0.65	0/2831	0.68	0/3859
All	All	0.65	0/5662	0.69	0/7718

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	306	TYR	Sidechain

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	2749	0	2709	257	3
1	B	2749	0	2709	327	2
2	A	39	0	34	1	0
3	B	50	0	43	0	0
4	A	28	0	25	0	0
4	B	28	0	25	1	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
6	A	4	0	0	0	1
6	B	3	0	0	0	1
7	A	20	0	27	2	0
7	B	20	0	27	2	0
8	A	50	0	89	7	0
8	B	50	0	89	4	0
9	B	10	0	16	1	0
10	A	38	0	52	3	0
10	B	38	0	52	4	1
11	A	37	0	0	6	0
11	B	29	0	0	10	0
All	All	5948	0	5897	584	4

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 50.

All (584) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:298:SER:HA	1:B:301:TYR:CE2	1.81	1.15
1:A:298:SER:HA	1:A:301:TYR:CE2	1.82	1.15
1:A:67:LYS:HB2	1:A:337:VAL:HB	1.38	1.02
1:B:64:GLN:HG3	1:B:339:LYS:HE2	1.39	1.02
1:A:345:VAL:HG12	1:A:347:PRO:HD3	1.45	0.98
1:B:337:VAL:HB	1:B:343:SER:HA	1.45	0.97
1:A:94:THR:HB	1:A:113:GLU:OE2	1.63	0.97
1:B:239:GLU:HB2	1:B:245:LYS:HD2	1.44	0.95
1:B:122:GLU:HG3	1:B:167:CYS:SG	2.06	0.94
1:A:65:HIS:ND1	1:A:338:SER:HA	1.81	0.94
1:A:88:PHE:HB3	8:B:1323:PLM:HB1	1.49	0.94
1:A:50:LEU:HD21	1:B:50:LEU:HB2	1.50	0.93
1:B:245:LYS:HA	1:B:245:LYS:HE3	1.51	0.92
1:A:239:GLU:HG2	1:A:248:LYS:NZ	1.85	0.91
1:B:298:SER:HB2	11:B:2036:HOH:O	1.73	0.88
1:B:245:LYS:NZ	1:B:248:LYS:HD2	1.91	0.86
1:A:316:CYS:SG	1:A:337:VAL:HG13	2.15	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:332:GLU:C	1:A:334:SER:H	1.77	0.85
1:B:183:MET:HE3	1:B:289:THR:HG21	1.57	0.84
1:A:65:HIS:HB3	1:A:337:VAL:HG22	1.60	0.84
1:B:157:VAL:O	1:B:161:TRP:HB2	1.78	0.83
1:B:346:ALA:N	1:B:347:PRO:HD3	1.93	0.83
1:B:298:SER:HA	1:B:301:TYR:HE2	1.40	0.83
1:A:298:SER:HA	1:A:301:TYR:CD2	2.14	0.83
1:B:271:VAL:HG21	1:B:291:PRO:HG3	1.61	0.82
1:B:72:LEU:HD22	1:B:250:VAL:HG13	1.59	0.82
1:B:67:LYS:HB3	1:B:337:VAL:CG1	2.10	0.82
1:B:267:PRO:HG2	11:B:2019:HOH:O	1.80	0.81
1:B:210:VAL:HA	1:B:214:ILE:HD12	1.60	0.81
1:A:341:GLU:CG	1:A:342:THR:H	1.94	0.81
1:A:77:LEU:O	1:A:81:VAL:HG23	1.80	0.81
7:A:1296:RET:H181	7:A:1296:RET:H8	1.63	0.80
1:A:307:ILE:O	1:A:307:ILE:HG22	1.80	0.80
1:A:298:SER:HA	1:A:301:TYR:HE2	1.42	0.80
1:A:326:ASN:O	1:A:328:LEU:HD22	1.83	0.79
1:A:239:GLU:HG2	1:A:248:LYS:HZ1	1.46	0.79
1:B:87:VAL:HA	1:B:91:PHE:HB2	1.65	0.79
1:A:90:GLY:O	1:A:94:THR:HG22	1.83	0.78
1:A:253:MET:HE1	1:A:306:TYR:HA	1.65	0.78
1:A:341:GLU:HG3	1:A:342:THR:N	1.98	0.77
1:B:312:GLN:HA	1:B:332:GLU:HG2	1.65	0.77
1:A:170:PRO:HB2	1:A:171:PRO:HD3	1.65	0.77
1:A:161:TRP:O	1:A:165:LEU:HB2	1.84	0.77
1:A:267:PRO:HG2	11:A:964:HOH:O	1.84	0.77
1:B:67:LYS:HE3	1:B:312:GLN:HG3	1.67	0.77
1:A:245:LYS:HZ2	1:A:245:LYS:HA	1.49	0.77
1:A:245:LYS:NZ	1:A:245:LYS:HA	2.00	0.77
1:A:87:VAL:O	1:A:91:PHE:HB2	1.85	0.76
1:B:214:ILE:HB	1:B:215:PRO:HD3	1.67	0.76
1:A:112:LEU:HD22	1:A:116:PHE:HE2	1.51	0.76
1:B:332:GLU:HB3	1:B:335:THR:O	1.85	0.76
1:B:248:LYS:O	1:B:252:ARG:HG3	1.83	0.76
1:B:338:SER:HB2	1:B:341:GLU:HG3	1.66	0.76
1:A:345:VAL:HG12	1:A:347:PRO:CD	2.16	0.75
1:B:209:VAL:HA	1:B:213:ILE:HB	1.68	0.75
1:B:67:LYS:H	1:B:337:VAL:CG2	2.00	0.75
1:A:266:LEU:N	1:A:267:PRO:HD2	2.02	0.74
1:A:67:LYS:HB2	1:A:337:VAL:CB	2.15	0.73
1:B:213:ILE:O	1:B:217:ILE:HG13	1.87	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:230:VAL:HG23	1:B:248:LYS:HD3	1.70	0.73
1:A:308:MET:HE1	1:B:42:ALA:N	2.04	0.73
1:B:337:VAL:HA	1:B:342:THR:O	1.89	0.72
1:B:139:VAL:HG11	1:B:230:VAL:HG12	1.71	0.72
1:A:253:MET:CE	1:A:306:TYR:HA	2.19	0.72
1:B:96:TYR:HE2	1:B:104:VAL:CG2	2.03	0.72
1:B:337:VAL:CB	1:B:343:SER:HA	2.19	0.72
1:B:94:THR:CG2	1:B:113:GLU:HG2	2.19	0.72
1:A:341:GLU:OE1	1:A:342:THR:HG22	1.88	0.72
1:A:150:GLU:O	1:A:154:ILE:HG13	1.90	0.72
1:A:85:PHE:O	1:A:89:GLY:HA3	1.89	0.71
1:A:325:LYS:HE3	1:A:341:GLU:OE1	1.90	0.71
7:B:1296:RET:H181	7:B:1296:RET:H8	1.73	0.71
1:B:126:TRP:CH2	1:B:215:PRO:HG3	2.25	0.71
1:B:234:ALA:HA	1:B:245:LYS:NZ	2.05	0.71
1:A:100:HIS:CE1	10:B:1509:HTG:O6	2.44	0.71
1:A:212:PHE:C	1:A:215:PRO:HD2	2.11	0.71
1:B:237:GLN:NE2	1:B:237:GLN:H	1.89	0.71
1:A:341:GLU:HG3	1:A:342:THR:H	1.55	0.70
1:A:302:ASN:HB2	11:A:2017:HOH:O	1.89	0.70
1:B:303:PRO:O	1:B:307:ILE:HG13	1.91	0.70
1:A:254:VAL:O	1:A:258:VAL:HG23	1.90	0.70
1:A:326:ASN:HD21	1:A:328:LEU:HD11	1.55	0.70
1:B:67:LYS:N	1:B:337:VAL:HG21	2.06	0.70
1:B:74:TYR:HE2	1:B:150:GLU:HG2	1.57	0.70
1:B:195:HIS:HB3	1:B:200:ASN:ND2	2.07	0.70
1:B:64:GLN:HG3	1:B:339:LYS:HB2	1.74	0.69
1:B:301:TYR:HE1	11:B:2008:HOH:O	1.75	0.69
1:B:257:MET:HG2	1:B:305:ILE:HG21	1.74	0.69
1:B:64:GLN:CG	1:B:339:LYS:HB2	2.22	0.69
1:B:77:LEU:O	1:B:81:VAL:HG23	1.92	0.69
1:B:307:ILE:HG22	1:B:307:ILE:O	1.92	0.69
1:A:67:LYS:H	1:A:337:VAL:HG23	1.57	0.69
1:B:338:SER:HB2	1:B:341:GLU:CG	2.23	0.69
1:B:59:LEU:O	1:B:63:VAL:HG23	1.93	0.68
1:B:54:ILE:HD11	1:B:303:PRO:HB2	1.73	0.68
1:B:169:ALA:HB3	1:B:170:PRO:HD3	1.75	0.68
1:B:239:GLU:HB3	1:B:244:GLN:HE22	1.59	0.68
1:B:59:LEU:HD12	1:B:77:LEU:HD11	1.75	0.68
1:A:212:PHE:O	1:A:215:PRO:HD2	1.94	0.68
1:B:337:VAL:HA	1:B:342:THR:C	2.13	0.68
1:B:337:VAL:HG23	1:B:338:SER:N	2.09	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:129:VAL:HG13	1:B:218:VAL:HG11	1.74	0.68
1:B:143:MET:HG2	1:B:146:PHE:HB3	1.76	0.68
1:A:65:HIS:ND1	1:A:337:VAL:O	2.27	0.68
1:A:167:CYS:HB2	1:A:207:MET:SD	2.34	0.68
1:B:238:GLN:HG3	1:B:241:ALA:H	1.59	0.68
1:B:143:MET:HG2	1:B:146:PHE:CB	2.24	0.67
1:A:191:TYR:O	1:A:279:GLN:HG2	1.93	0.67
1:A:341:GLU:CG	1:A:342:THR:N	2.57	0.67
1:B:94:THR:HG22	1:B:113:GLU:CG	2.25	0.67
1:B:94:THR:HG22	1:B:113:GLU:HG2	1.75	0.67
1:A:213:ILE:O	1:A:217:ILE:HG12	1.93	0.67
1:A:75:ILE:O	1:A:79:LEU:HB2	1.95	0.67
1:B:332:GLU:OE2	1:B:334:SER:HB2	1.94	0.67
1:A:332:GLU:C	1:A:334:SER:N	2.49	0.66
1:B:129:VAL:CG1	1:B:218:VAL:HG11	2.25	0.66
1:A:70:THR:H	1:A:73:ASN:HD22	1.42	0.66
1:B:129:VAL:HG13	1:B:218:VAL:CG1	2.26	0.66
1:A:181:GLU:OE2	1:A:188:GLY:HA3	1.96	0.66
1:B:65:HIS:HB2	1:B:68:LEU:HD12	1.77	0.66
1:A:239:GLU:HG2	1:A:248:LYS:HZ2	1.61	0.66
1:B:54:ILE:CD1	1:B:303:PRO:HB2	2.25	0.66
1:B:67:LYS:HB3	1:B:337:VAL:HG11	1.78	0.65
1:B:67:LYS:HD3	1:B:337:VAL:HG13	1.78	0.65
1:A:97:THR:HG21	1:A:185:CYS:HA	1.77	0.65
1:A:238:GLN:HA	1:A:242:THR:HA	1.79	0.65
1:A:137:VAL:HA	1:A:142:PRO:CD	2.27	0.65
1:A:239:GLU:HB3	1:A:244:GLN:CD	2.17	0.65
1:B:266:LEU:N	1:B:267:PRO:HD2	2.11	0.65
1:A:325:LYS:HE2	1:A:327:PRO:HD3	1.79	0.65
1:A:99:LEU:HD11	10:B:1509:HTG:H3'1	1.77	0.65
1:B:237:GLN:O	1:B:238:GLN:HB3	1.97	0.65
1:A:103:PHE:CE2	1:A:180:PRO:HB3	2.31	0.65
1:A:300:VAL:O	1:A:302:ASN:N	2.30	0.64
1:A:97:THR:CG2	1:A:185:CYS:HA	2.27	0.64
1:A:338:SER:HB2	1:A:341:GLU:HG2	1.79	0.64
1:B:67:LYS:HZ1	1:B:332:GLU:HG3	1.63	0.64
1:B:195:HIS:CE1	1:B:197:GLU:HB3	2.32	0.64
1:B:85:PHE:O	1:B:89:GLY:N	2.29	0.64
1:B:131:LEU:HD23	1:B:254:VAL:HG13	1.80	0.63
1:B:238:GLN:HA	1:B:242:THR:HA	1.79	0.63
1:A:337:VAL:O	1:A:338:SER:OG	2.17	0.63
1:A:235:ALA:HB3	1:A:239:GLU:OE1	1.98	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:103:PHE:CZ	1:A:187:CYS:SG	2.92	0.63
1:A:326:ASN:OD1	1:A:328:LEU:HD13	1.99	0.63
1:A:110:CYS:HB3	11:A:2045:HOH:O	1.99	0.63
1:A:227:VAL:HG13	1:A:228:PHE:N	2.13	0.63
1:B:199:ASN:ND2	11:B:2005:HOH:O	2.31	0.62
1:A:283:PHE:HB2	1:A:287:PHE:CD2	2.35	0.62
1:A:303:PRO:O	1:A:307:ILE:HG13	2.00	0.62
1:A:271:VAL:HG21	1:A:291:PRO:HG3	1.80	0.62
1:A:304:VAL:O	1:A:308:MET:CG	2.47	0.62
1:A:322:CYS:O	1:A:324:GLY:N	2.32	0.62
1:A:57:LEU:HD23	8:A:1322:PLM:HD2	1.81	0.62
1:A:96:TYR:HE2	1:A:104:VAL:HG21	1.65	0.61
1:B:6:GLY:HA3	1:B:9:PHE:CZ	2.34	0.61
1:B:150:GLU:O	1:B:154:ILE:HD13	2.00	0.61
1:A:35:TRP:HZ3	1:A:39:MET:SD	2.23	0.61
1:A:342:THR:O	1:A:342:THR:HG23	2.01	0.61
1:A:234:ALA:HB2	1:A:248:LYS:HG2	1.82	0.61
1:A:75:ILE:HG21	1:A:131:LEU:HD13	1.82	0.61
1:B:96:TYR:HE2	1:B:104:VAL:HG22	1.66	0.61
1:B:236:GLN:HB2	1:B:237:GLN:NE2	2.15	0.61
1:B:302:ASN:HB2	11:B:2016:HOH:O	2.00	0.61
1:B:337:VAL:HB	1:B:343:SER:CA	2.26	0.60
1:A:67:LYS:H	1:A:337:VAL:CG2	2.13	0.60
1:B:113:GLU:OE1	1:B:187:CYS:HB2	2.01	0.60
1:A:224:GLY:O	1:A:227:VAL:HG12	2.01	0.60
1:B:76:LEU:HD13	1:B:306:TYR:CG	2.36	0.60
1:A:65:HIS:HB3	1:A:337:VAL:CG2	2.31	0.60
1:A:253:MET:HE1	1:A:306:TYR:HD1	1.67	0.60
1:A:180:PRO:HA	1:A:186:SER:O	2.00	0.60
1:A:312:GLN:NE2	1:A:337:VAL:HG12	2.16	0.60
1:A:59:LEU:O	1:A:59:LEU:HD12	2.01	0.60
1:B:327:PRO:HB2	1:B:331:ASP:OD2	2.02	0.60
1:B:75:ILE:HG13	1:B:131:LEU:CD1	2.32	0.60
1:B:143:MET:HA	1:B:143:MET:CE	2.32	0.60
1:A:93:THR:O	1:A:96:TYR:N	2.34	0.59
1:A:59:LEU:HD13	1:A:77:LEU:HD11	1.84	0.59
1:B:96:TYR:HE2	1:B:104:VAL:HG21	1.67	0.59
1:B:54:ILE:HG23	1:B:55:ASN:N	2.17	0.59
1:B:195:HIS:HB3	1:B:200:ASN:HD21	1.67	0.59
1:B:64:GLN:HG3	1:B:339:LYS:CE	2.24	0.59
1:A:137:VAL:HA	1:A:142:PRO:HD2	1.85	0.59
1:A:65:HIS:ND1	1:A:338:SER:CA	2.61	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:66:LYS:HD2	1:A:66:LYS:N	2.18	0.59
1:B:46:LEU:HD12	8:B:1407:PLM:HD2	1.85	0.59
1:B:67:LYS:HB3	1:B:337:VAL:CG2	2.32	0.59
1:B:122:GLU:HA	1:B:122:GLU:OE1	2.02	0.59
1:B:143:MET:HA	1:B:143:MET:HE2	1.84	0.59
1:A:307:ILE:CG2	1:A:307:ILE:O	2.51	0.59
1:B:119:LEU:HD23	1:B:120:GLY:N	2.17	0.59
1:B:245:LYS:HZ1	1:B:248:LYS:HD2	1.68	0.58
1:A:239:GLU:HB3	1:A:244:GLN:NE2	2.18	0.58
1:A:212:PHE:HB2	7:A:1296:RET:H32	1.84	0.58
1:B:220:PHE:O	1:B:223:TYR:HB3	2.04	0.58
1:B:183:MET:CE	1:B:289:THR:HG21	2.32	0.58
1:A:210:VAL:HG12	1:A:210:VAL:O	2.02	0.58
1:B:67:LYS:NZ	1:B:332:GLU:HG3	2.17	0.58
1:A:304:VAL:O	1:A:308:MET:HG2	2.04	0.58
1:B:67:LYS:NZ	1:B:336:THR:HA	2.18	0.58
1:B:234:ALA:HB1	1:B:245:LYS:HE2	1.86	0.58
1:B:241:ALA:HB1	1:B:243:THR:HG22	1.86	0.58
1:A:6:GLY:HA3	1:A:9:PHE:CZ	2.38	0.58
1:B:36:GLN:O	1:B:39:MET:HB2	2.04	0.58
1:A:178:TYR:HA	1:A:188:GLY:O	2.04	0.57
1:B:332:GLU:O	1:B:333:ALA:HB3	2.04	0.57
1:A:218:VAL:O	1:A:218:VAL:HG12	2.04	0.57
1:B:180:PRO:HG2	11:B:2023:HOH:O	2.03	0.57
1:B:302:ASN:HB2	1:B:303:PRO:HD3	1.86	0.57
1:B:48:ILE:HD12	1:B:95:LEU:HD22	1.85	0.57
1:A:192:TYR:O	1:A:279:GLN:HB3	2.03	0.57
1:A:189:ILE:CG2	1:A:190:ASP:N	2.68	0.57
1:A:326:ASN:ND2	1:A:328:LEU:HD21	2.19	0.56
1:B:312:GLN:HA	1:B:332:GLU:CG	2.34	0.56
1:B:239:GLU:HB3	1:B:244:GLN:NE2	2.19	0.56
1:B:326:ASN:O	1:B:328:LEU:HD22	2.04	0.56
1:B:283:PHE:N	1:B:283:PHE:CD1	2.74	0.56
1:B:67:LYS:HZ2	1:B:336:THR:HA	1.70	0.56
1:B:239:GLU:HB2	1:B:245:LYS:CD	2.28	0.56
1:B:92:THR:O	1:B:95:LEU:HB3	2.05	0.56
1:B:170:PRO:HB2	1:B:171:PRO:HD3	1.88	0.56
1:B:259:ILE:HG22	1:B:263:ILE:HD12	1.85	0.56
1:A:250:VAL:O	1:A:254:VAL:HG23	2.04	0.56
1:A:65:HIS:HB2	1:A:68:LEU:HD12	1.86	0.56
1:B:226:LEU:HD12	1:B:226:LEU:N	2.20	0.56
1:B:167:CYS:HB2	1:B:211:HIS:NE2	2.21	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:70:THR:HG23	1:A:73:ASN:ND2	2.21	0.56
1:A:175:TRP:CZ2	1:A:203:PHE:HA	2.41	0.56
1:A:298:SER:CA	1:A:301:TYR:CE2	2.75	0.56
1:A:230:VAL:HG23	1:A:248:LYS:HE2	1.88	0.56
1:B:298:SER:HA	1:B:301:TYR:CD2	2.37	0.55
1:B:129:VAL:HG22	1:B:219:ILE:HG13	1.88	0.55
1:B:244:GLN:O	1:B:248:LYS:HG3	2.05	0.55
1:B:345:VAL:C	1:B:347:PRO:HD3	2.26	0.55
8:A:1322:PLM:H61	1:B:88:PHE:HE1	1.69	0.55
1:A:346:ALA:N	1:A:347:PRO:HD3	2.21	0.55
1:B:234:ALA:HA	1:B:245:LYS:HZ3	1.71	0.55
1:B:245:LYS:CE	1:B:248:LYS:HD2	2.36	0.55
1:A:338:SER:CB	1:A:341:GLU:HG2	2.36	0.55
1:B:57:LEU:HD21	1:B:321:LEU:HD21	1.89	0.55
1:B:326:ASN:HB3	1:B:328:LEU:CD2	2.37	0.55
1:B:33:GLU:HB2	1:B:36:GLN:HG3	1.89	0.55
1:B:212:PHE:O	1:B:216:LEU:HD23	2.07	0.54
1:B:208:PHE:O	1:B:213:ILE:HD12	2.06	0.54
1:A:103:PHE:HE2	1:A:180:PRO:HB3	1.70	0.54
1:B:135:ARG:HA	1:B:135:ARG:NE	2.22	0.54
1:A:311:LYS:HG2	1:A:331:ASP:O	2.06	0.54
1:B:337:VAL:HA	1:B:342:THR:HG23	1.90	0.54
1:B:78:ASN:O	1:B:81:VAL:N	2.40	0.54
1:A:267:PRO:O	1:A:271:VAL:HG23	2.07	0.54
1:B:143:MET:CG	1:B:146:PHE:HB3	2.37	0.54
1:B:136:TYR:HA	1:B:226:LEU:HD11	1.88	0.54
1:B:238:GLN:HG3	1:B:241:ALA:N	2.21	0.54
1:A:79:LEU:HD11	1:A:124:ALA:HA	1.90	0.54
1:A:267:PRO:HA	10:A:1507:HTG:H6'1	1.90	0.54
1:B:67:LYS:CE	1:B:312:GLN:HG3	2.35	0.54
1:B:234:ALA:HA	1:B:245:LYS:HZ2	1.73	0.54
1:A:139:VAL:HG11	1:A:226:LEU:HG	1.90	0.54
1:A:157:VAL:O	1:A:161:TRP:HD1	1.91	0.54
1:B:237:GLN:H	1:B:237:GLN:HE21	1.55	0.53
1:A:332:GLU:O	1:A:334:SER:N	2.42	0.53
1:A:237:GLN:O	1:A:238:GLN:HB3	2.07	0.53
1:A:232:GLU:HA	1:A:252:ARG:HD3	1.91	0.53
1:A:85:PHE:O	1:A:89:GLY:CA	2.57	0.53
1:B:288:MET:HG3	1:B:288:MET:O	2.06	0.53
1:A:227:VAL:CG1	1:A:228:PHE:N	2.71	0.53
1:A:311:LYS:CE	1:A:330:ASP:HB2	2.38	0.53
1:B:245:LYS:HZ3	1:B:248:LYS:HD2	1.71	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:326:ASN:C	1:B:328:LEU:HD22	2.29	0.53
1:B:263:ILE:O	1:B:294:PHE:HE2	1.92	0.53
1:B:54:ILE:O	1:B:57:LEU:HB3	2.09	0.53
1:A:266:LEU:N	1:A:267:PRO:CD	2.71	0.53
1:A:311:LYS:O	1:A:315:ASN:ND2	2.40	0.53
1:B:283:PHE:HB2	1:B:287:PHE:CD2	2.44	0.53
1:B:64:GLN:HG2	1:B:339:LYS:HB2	1.91	0.53
1:B:322:CYS:HA	8:B:1322:PLM:O1	2.08	0.53
1:A:53:PRO:O	1:A:57:LEU:HB2	2.09	0.53
1:B:139:VAL:HG21	1:B:226:LEU:HD23	1.92	0.52
1:B:238:GLN:HG3	1:B:241:ALA:CA	2.39	0.52
1:B:332:GLU:CB	1:B:335:THR:O	2.57	0.52
1:B:235:ALA:HB3	1:B:239:GLU:OE1	2.09	0.52
1:A:300:VAL:O	1:A:303:PRO:HD2	2.08	0.52
1:A:321:LEU:HD13	8:A:1322:PLM:H72	1.91	0.52
1:B:283:PHE:HB2	1:B:287:PHE:HD2	1.73	0.52
1:B:286:ILE:O	1:B:290:ILE:HG12	2.09	0.52
1:B:221:PHE:O	1:B:224:GLY:N	2.37	0.52
1:A:96:TYR:CE2	1:A:104:VAL:HG21	2.43	0.52
1:B:139:VAL:CG1	1:B:230:VAL:HG12	2.39	0.52
1:B:207:MET:SD	1:B:211:HIS:HD2	2.33	0.52
1:B:103:PHE:CZ	1:B:187:CYS:SG	3.03	0.52
1:B:32:ALA:HB1	1:B:36:GLN:OE1	2.10	0.52
1:A:158:ALA:O	1:A:162:VAL:HG23	2.10	0.52
1:B:337:VAL:CA	1:B:342:THR:HG23	2.40	0.52
1:B:129:VAL:HG22	1:B:219:ILE:CG1	2.40	0.52
1:A:237:GLN:CD	1:A:237:GLN:H	2.14	0.51
1:A:156:GLY:O	1:A:159:PHE:HB3	2.10	0.51
1:B:129:VAL:C	1:B:131:LEU:N	2.64	0.51
1:A:133:ILE:O	1:A:136:TYR:N	2.44	0.51
1:B:332:GLU:OE1	1:B:332:GLU:O	2.29	0.51
1:A:139:VAL:HG11	1:A:230:VAL:HG12	1.91	0.51
1:A:169:ALA:N	1:A:170:PRO:CD	2.73	0.51
1:B:146:PHE:HE1	1:B:152:HIS:NE2	2.09	0.51
2:A:504:NAG:C7	2:A:505:NAG:H61	2.40	0.51
1:B:67:LYS:HZ2	1:B:335:THR:C	2.14	0.51
1:B:284:GLY:O	1:B:287:PHE:HB3	2.10	0.51
1:B:239:GLU:CB	1:B:244:GLN:HE22	2.23	0.51
1:A:300:VAL:C	1:A:302:ASN:H	2.14	0.51
1:B:171:PRO:HA	1:B:175:TRP:O	2.11	0.51
1:B:35:TRP:O	1:B:39:MET:HG2	2.11	0.51
1:B:50:LEU:C	1:B:50:LEU:CD2	2.79	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:171:PRO:HG2	1:B:189:ILE:HD11	1.92	0.50
1:B:230:VAL:HG23	1:B:248:LYS:CD	2.39	0.50
1:A:239:GLU:HB3	1:A:244:GLN:OE1	2.10	0.50
1:A:251:THR:C	1:A:253:MET:N	2.64	0.50
8:A:1322:PLM:H91	1:B:49:MET:SD	2.51	0.50
1:B:170:PRO:HB3	1:B:175:TRP:HB3	1.94	0.50
1:A:110:CYS:SG	1:A:180:PRO:HD3	2.51	0.50
1:A:52:PHE:HB3	1:A:53:PRO:CD	2.42	0.50
1:A:67:LYS:HB2	1:A:337:VAL:CG2	2.42	0.50
1:A:36:GLN:O	1:A:39:MET:HB2	2.11	0.50
1:A:44:MET:HB2	1:A:95:LEU:HD13	1.94	0.50
1:A:104:VAL:C	1:A:106:GLY:H	2.16	0.50
1:A:77:LEU:O	1:A:77:LEU:HD12	2.12	0.50
1:A:308:MET:HE1	1:B:41:ALA:C	2.32	0.50
1:B:330:ASP:O	1:B:331:ASP:O	2.29	0.50
1:A:59:LEU:O	1:A:63:VAL:HG23	2.12	0.50
1:A:304:VAL:O	1:A:308:MET:HG3	2.11	0.49
1:B:64:GLN:HA	1:B:339:LYS:HD3	1.93	0.49
1:B:123:ILE:HG13	1:B:164:ALA:HB3	1.94	0.49
1:A:247:GLU:HA	1:A:247:GLU:OE1	2.11	0.49
1:B:301:TYR:O	1:B:305:ILE:HG13	2.12	0.49
1:B:340:THR:HG23	1:B:341:GLU:N	2.27	0.49
1:B:67:LYS:HZ2	1:B:336:THR:CA	2.25	0.49
1:B:346:ALA:N	1:B:347:PRO:CD	2.71	0.49
1:A:88:PHE:HA	1:A:92:THR:HG23	1.94	0.49
1:B:129:VAL:C	1:B:131:LEU:H	2.15	0.49
1:A:286:ILE:O	1:A:290:ILE:HG12	2.13	0.49
1:A:283:PHE:HB2	1:A:287:PHE:HD2	1.76	0.49
1:B:227:VAL:HG13	1:B:228:PHE:N	2.26	0.49
1:A:139:VAL:HG21	1:A:230:VAL:HG11	1.95	0.49
1:A:276:PHE:O	1:A:279:GLN:HG3	2.13	0.49
1:B:227:VAL:CG1	1:B:228:PHE:N	2.75	0.49
1:B:239:GLU:HB3	1:B:244:GLN:OE1	2.13	0.49
1:B:133:ILE:N	1:B:133:ILE:HD13	2.28	0.49
1:B:67:LYS:N	1:B:337:VAL:CG2	2.66	0.48
1:A:42:ALA:O	1:A:45:PHE:HB3	2.13	0.48
1:A:91:PHE:HA	1:A:94:THR:CG2	2.43	0.48
1:B:78:ASN:OD1	1:B:157:VAL:HG13	2.12	0.48
9:B:1401:HTO:H72	10:B:1509:HTG:H3'2	1.95	0.48
1:A:240:SER:O	1:A:241:ALA:HB2	2.12	0.48
1:A:12:PRO:HD3	11:A:2064:HOH:O	2.11	0.48
1:B:265:TRP:C	1:B:267:PRO:HD2	2.33	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:321:LEU:C	1:A:323:CYS:H	2.16	0.48
1:B:93:THR:O	1:B:96:TYR:HB3	2.12	0.48
1:B:78:ASN:O	1:B:79:LEU:C	2.51	0.48
1:A:245:LYS:NZ	1:A:245:LYS:CA	2.76	0.48
1:B:282:ASP:HB2	4:B:805:NAG:H62	1.96	0.48
1:A:153:ALA:O	1:A:157:VAL:HG23	2.13	0.48
1:B:104:VAL:C	1:B:106:GLY:H	2.17	0.48
1:B:283:PHE:HD1	1:B:283:PHE:H	1.59	0.48
1:B:259:ILE:C	1:B:261:PHE:H	2.17	0.48
1:B:123:ILE:HG13	1:B:164:ALA:CB	2.44	0.48
1:B:67:LYS:HB3	1:B:337:VAL:HG13	1.91	0.48
1:A:126:TRP:NE1	1:A:163:MET:HB3	2.28	0.48
1:A:302:ASN:CB	1:A:303:PRO:HD3	2.43	0.48
1:B:281:SER:OG	1:B:282:ASP:N	2.47	0.48
1:B:136:TYR:CE2	1:B:142:PRO:HG2	2.49	0.48
1:B:321:LEU:C	1:B:323:CYS:H	2.16	0.48
1:A:135:ARG:HA	1:A:135:ARG:NE	2.29	0.48
1:B:126:TRP:NE1	1:B:163:MET:HB3	2.29	0.47
1:A:232:GLU:HB3	1:A:252:ARG:HD3	1.96	0.47
1:B:151:ASN:HD21	1:B:152:HIS:CE1	2.32	0.47
1:B:261:PHE:C	1:B:263:ILE:H	2.17	0.47
1:B:280:GLY:O	1:B:281:SER:O	2.32	0.47
1:A:311:LYS:HE3	1:A:331:ASP:O	2.15	0.47
1:B:238:GLN:HB2	1:B:242:THR:OG1	2.14	0.47
1:B:67:LYS:HD3	1:B:336:THR:C	2.35	0.47
1:A:59:LEU:C	1:A:59:LEU:HD12	2.34	0.47
1:A:311:LYS:NZ	1:A:330:ASP:HB2	2.29	0.47
1:B:67:LYS:H	1:B:337:VAL:HG22	1.77	0.47
1:A:94:THR:HB	1:A:113:GLU:CD	2.30	0.47
1:B:126:TRP:HA	1:B:126:TRP:CE3	2.48	0.47
1:A:175:TRP:NE1	1:A:203:PHE:HB2	2.29	0.47
1:A:298:SER:CA	1:A:301:TYR:HE2	2.20	0.47
1:B:238:GLN:HG3	1:B:241:ALA:C	2.34	0.47
1:B:240:SER:O	1:B:241:ALA:CB	2.62	0.47
1:A:232:GLU:CA	1:A:252:ARG:HD3	2.45	0.47
1:A:122:GLU:HG3	1:A:167:CYS:SG	2.54	0.47
1:B:200:ASN:HB3	11:B:2044:HOH:O	2.14	0.47
1:B:76:LEU:HD13	1:B:306:TYR:CD1	2.50	0.47
1:B:178:TYR:HA	1:B:188:GLY:O	2.15	0.47
1:B:126:TRP:CZ3	1:B:215:PRO:HG3	2.50	0.47
1:B:8:ASN:HA	1:B:8:ASN:HD22	1.50	0.47
1:A:278:HIS:O	1:A:280:GLY:N	2.48	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:64:GLN:HA	1:B:339:LYS:NZ	2.29	0.47
1:A:200:ASN:O	1:A:204:VAL:HG23	2.15	0.47
1:A:148:PHE:HA	1:A:152:HIS:ND1	2.30	0.47
1:B:154:ILE:HD12	1:B:154:ILE:N	2.30	0.46
1:B:328:LEU:O	1:B:329:GLY:C	2.53	0.46
8:B:1322:PLM:H52	8:B:1323:PLM:H61	1.97	0.46
1:A:170:PRO:CB	1:A:171:PRO:HD3	2.39	0.46
1:B:68:LEU:HB3	1:B:73:ASN:HD22	1.80	0.46
1:A:253:MET:HE1	1:A:306:TYR:CD1	2.50	0.46
1:A:231:LYS:HB2	1:A:231:LYS:NZ	2.30	0.46
1:B:341:GLU:OE1	1:B:342:THR:HG22	2.15	0.46
1:A:300:VAL:C	1:A:302:ASN:N	2.69	0.46
1:B:150:GLU:O	1:B:154:ILE:CD1	2.63	0.46
1:A:130:VAL:HG12	1:A:130:VAL:O	2.14	0.46
1:A:251:THR:O	1:A:253:MET:N	2.49	0.46
1:B:304:VAL:O	1:B:308:MET:HG3	2.16	0.46
1:B:58:THR:O	1:B:59:LEU:C	2.52	0.46
1:A:130:VAL:HG21	1:A:160:THR:CG2	2.45	0.46
1:A:70:THR:HG23	1:A:73:ASN:HD22	1.80	0.46
1:B:132:ALA:O	1:B:222:CYS:SG	2.70	0.46
1:B:336:THR:O	1:B:337:VAL:O	2.33	0.46
1:B:160:THR:O	1:B:162:VAL:N	2.49	0.46
1:B:165:LEU:C	1:B:167:CYS:H	2.19	0.46
1:A:267:PRO:HA	10:A:1507:HTG:C6'	2.45	0.46
1:A:231:LYS:HZ2	1:A:233:ALA:HB3	1.81	0.46
1:B:33:GLU:O	1:B:36:GLN:HB2	2.16	0.46
1:B:160:THR:C	1:B:162:VAL:H	2.20	0.45
1:A:251:THR:O	1:A:252:ARG:C	2.55	0.45
1:A:321:LEU:HD13	8:A:1322:PLM:H51	1.97	0.45
1:B:64:GLN:HA	1:B:339:LYS:HZ2	1.81	0.45
1:B:237:GLN:N	1:B:237:GLN:HE21	2.14	0.45
1:B:57:LEU:HD13	1:B:57:LEU:C	2.36	0.45
1:B:68:LEU:HA	1:B:73:ASN:ND2	2.32	0.45
1:B:244:GLN:OE1	1:B:248:LYS:HE2	2.16	0.45
1:A:88:PHE:HA	1:A:92:THR:CG2	2.47	0.45
1:B:129:VAL:CG2	1:B:219:ILE:HD11	2.47	0.45
1:A:74:TYR:CE2	1:A:150:GLU:HG2	2.52	0.45
1:A:137:VAL:O	1:A:141:LYS:HA	2.15	0.45
1:A:28:GLN:HB3	1:A:31:LEU:HD12	1.98	0.45
1:B:259:ILE:C	1:B:261:PHE:N	2.69	0.45
1:B:67:LYS:HZ2	1:B:336:THR:N	2.15	0.45
1:B:307:ILE:O	1:B:307:ILE:CG2	2.61	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:134:GLU:HG2	1:A:148:PHE:CD2	2.51	0.45
1:B:160:THR:C	1:B:162:VAL:N	2.70	0.45
1:A:290:ILE:HB	1:A:291:PRO:CD	2.47	0.45
1:B:119:LEU:C	1:B:119:LEU:HD23	2.36	0.45
1:B:65:HIS:NE2	1:B:320:THR:OG1	2.49	0.45
1:B:126:TRP:HB3	1:B:160:THR:HG22	1.97	0.45
1:B:33:GLU:HB3	1:B:35:TRP:CD1	2.52	0.45
1:B:237:GLN:O	1:B:238:GLN:CB	2.65	0.44
1:A:75:ILE:HG13	1:A:131:LEU:HD13	1.98	0.44
1:A:231:LYS:HB2	1:A:231:LYS:HZ2	1.81	0.44
1:A:312:GLN:HB2	1:A:332:GLU:HG3	1.99	0.44
1:A:134:GLU:HG2	1:A:148:PHE:CE2	2.53	0.44
1:A:305:ILE:HG12	10:A:1508:HTG:H6'2	1.99	0.44
1:B:67:LYS:HE2	1:B:316:CYS:SG	2.57	0.44
1:A:307:ILE:HG12	1:A:313:PHE:CE2	2.52	0.44
1:B:35:TRP:CZ3	1:B:39:MET:HG3	2.52	0.44
1:B:240:SER:O	1:B:241:ALA:HB2	2.18	0.44
1:A:256:ILE:HA	1:A:256:ILE:HD13	1.85	0.44
1:A:256:ILE:HG22	1:A:305:ILE:HD13	1.99	0.44
1:A:322:CYS:HA	8:A:1322:PLM:O1	2.17	0.44
1:B:264:CYS:SG	1:B:298:SER:HB3	2.57	0.44
1:A:264:CYS:SG	1:A:295:ALA:O	2.76	0.44
1:B:244:GLN:HE21	1:B:245:LYS:N	2.16	0.44
1:A:35:TRP:CZ3	1:A:39:MET:SD	3.08	0.44
1:A:326:ASN:ND2	1:A:328:LEU:CD2	2.81	0.44
1:A:342:THR:C	1:A:344:GLN:H	2.21	0.44
1:A:93:THR:HG22	1:A:94:THR:N	2.32	0.44
1:B:124:ALA:O	1:B:128:LEU:HG	2.17	0.44
1:B:167:CYS:SG	1:B:207:MET:CE	3.06	0.44
1:B:129:VAL:HG23	1:B:219:ILE:HD11	2.00	0.44
1:B:102:TYR:CE2	1:B:104:VAL:HA	2.53	0.44
1:B:148:PHE:CD1	1:B:152:HIS:HB2	2.52	0.44
1:B:44:MET:O	1:B:48:ILE:HG13	2.17	0.44
1:A:327:PRO:O	1:A:328:LEU:C	2.56	0.44
1:B:238:GLN:CG	1:B:241:ALA:H	2.29	0.44
1:B:143:MET:CB	1:B:146:PHE:HB3	2.48	0.44
1:A:259:ILE:C	1:A:261:PHE:H	2.21	0.44
1:A:338:SER:HB2	1:A:341:GLU:CG	2.47	0.43
1:A:301:TYR:HE1	11:A:2020:HOH:O	2.01	0.43
1:A:50:LEU:HD21	1:B:50:LEU:CB	2.36	0.43
1:B:171:PRO:HA	1:B:176:SER:O	2.18	0.43
1:A:115:PHE:O	1:A:118:THR:N	2.51	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:171:PRO:HG2	1:B:189:ILE:CD1	2.48	0.43
1:B:162:VAL:O	1:B:165:LEU:N	2.50	0.43
1:B:50:LEU:O	1:B:52:PHE:N	2.51	0.43
1:A:112:LEU:HD22	1:A:116:PHE:CE2	2.41	0.43
1:B:110:CYS:HB3	11:B:2060:HOH:O	2.18	0.43
1:B:262:LEU:HB3	1:B:266:LEU:HD22	2.00	0.43
1:B:189:ILE:HG22	1:B:190:ASP:N	2.32	0.43
1:A:137:VAL:O	1:A:137:VAL:HG12	2.17	0.43
1:A:224:GLY:O	1:A:227:VAL:CG1	2.66	0.43
1:B:221:PHE:CD1	1:B:221:PHE:C	2.92	0.43
1:A:314:ARG:O	1:A:317:MET:HB3	2.19	0.43
1:B:156:GLY:HA2	1:B:159:PHE:HB3	2.00	0.43
1:A:336:THR:C	1:A:337:VAL:HG12	2.38	0.43
1:A:268:TYR:HA	1:A:291:PRO:HB2	1.99	0.43
1:B:85:PHE:O	1:B:89:GLY:CA	2.65	0.43
1:A:199:ASN:HB3	1:A:202:SER:OG	2.19	0.43
1:A:338:SER:OG	1:A:341:GLU:OE2	2.34	0.43
1:A:264:CYS:SG	1:A:298:SER:HB3	2.59	0.43
1:A:238:GLN:HA	1:A:242:THR:CA	2.48	0.43
1:B:96:TYR:CE2	1:B:104:VAL:HG21	2.51	0.43
1:A:262:LEU:HB3	1:A:266:LEU:HD22	2.01	0.42
1:B:54:ILE:CG2	1:B:55:ASN:N	2.81	0.42
1:B:106:GLY:HA3	1:B:107:PRO:HD2	1.89	0.42
1:B:152:HIS:O	1:B:155:MET:HB2	2.20	0.42
1:B:47:LEU:HA	1:B:47:LEU:HD23	1.86	0.42
1:B:22:SER:C	1:B:24:PHE:H	2.22	0.42
1:B:193:THR:HA	1:B:194:PRO:HD3	1.92	0.42
1:B:183:MET:CE	1:B:286:ILE:HD13	2.49	0.42
1:B:266:LEU:N	1:B:267:PRO:CD	2.79	0.42
1:A:56:PHE:O	1:A:59:LEU:HB3	2.19	0.42
1:A:49:MET:SD	1:B:54:ILE:HB	2.59	0.42
1:B:189:ILE:CG2	1:B:190:ASP:N	2.81	0.42
1:B:288:MET:CG	1:B:288:MET:O	2.68	0.42
1:A:8:ASN:HA	1:A:8:ASN:HD22	1.50	0.42
1:A:330:ASP:OD2	1:B:100:HIS:CE1	2.72	0.42
1:B:65:HIS:N	1:B:65:HIS:CD2	2.87	0.42
1:A:238:GLN:HG2	1:A:239:GLU:N	2.34	0.42
1:A:167:CYS:C	1:A:170:PRO:HD2	2.40	0.42
1:A:227:VAL:CG1	1:A:228:PHE:H	2.32	0.42
1:A:218:VAL:O	1:A:218:VAL:CG1	2.67	0.42
1:B:259:ILE:O	1:B:261:PHE:N	2.52	0.42
1:B:115:PHE:CD1	1:B:172:LEU:HD11	2.54	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:255:ILE:HG22	1:B:256:ILE:N	2.34	0.42
1:B:209:VAL:O	1:B:214:ILE:HG13	2.19	0.42
1:A:253:MET:HE3	1:A:306:TYR:HA	1.99	0.42
1:B:85:PHE:O	1:B:89:GLY:HA3	2.20	0.42
1:B:134:GLU:CD	1:B:135:ARG:HH21	2.22	0.42
1:B:224:GLY:O	1:B:227:VAL:HG12	2.19	0.42
1:A:99:LEU:HD23	1:A:99:LEU:HA	1.79	0.42
1:A:44:MET:O	1:A:48:ILE:HG13	2.20	0.42
1:B:183:MET:HE1	1:B:286:ILE:HD13	2.02	0.42
1:A:115:PHE:O	1:A:116:PHE:C	2.56	0.42
1:B:199:ASN:HB3	11:B:2005:HOH:O	2.19	0.42
1:A:124:ALA:HB2	11:A:2030:HOH:O	2.20	0.42
1:A:225:GLN:C	1:A:227:VAL:H	2.21	0.42
1:A:35:TRP:O	1:A:38:SER:HB2	2.20	0.42
1:B:250:VAL:O	1:B:254:VAL:HG23	2.20	0.42
1:B:171:PRO:HG3	1:B:176:SER:HB3	2.02	0.42
1:B:191:TYR:CE2	1:B:272:ALA:HB1	2.55	0.42
1:B:301:TYR:CD1	1:B:301:TYR:C	2.93	0.41
1:B:167:CYS:HB2	1:B:211:HIS:CD2	2.55	0.41
1:A:239:GLU:CG	1:A:248:LYS:HZ2	2.31	0.41
1:B:146:PHE:CE1	1:B:152:HIS:NE2	2.86	0.41
1:A:40:LEU:O	1:A:44:MET:HG2	2.20	0.41
1:A:345:VAL:CG1	1:A:347:PRO:HD3	2.33	0.41
7:B:1296:RET:H201	11:B:2018:HOH:O	2.20	0.41
1:B:135:ARG:NH2	1:B:138:VAL:HG21	2.35	0.41
1:B:50:LEU:HD23	1:B:50:LEU:C	2.41	0.41
1:B:129:VAL:O	1:B:133:ILE:HG12	2.20	0.41
1:A:126:TRP:CH2	1:A:215:PRO:HG3	2.55	0.41
1:A:22:SER:C	1:A:24:PHE:H	2.22	0.41
1:B:276:PHE:O	1:B:279:GLN:HG3	2.21	0.41
1:A:347:PRO:HB2	1:A:348:ALA:H	1.58	0.41
1:A:62:THR:CG2	1:A:77:LEU:HD22	2.49	0.41
1:A:337:VAL:CG2	1:A:338:SER:N	2.83	0.41
1:B:68:LEU:CA	1:B:73:ASN:HD22	2.34	0.41
1:B:338:SER:CB	1:B:341:GLU:CD	2.88	0.41
1:B:322:CYS:O	1:B:324:GLY:N	2.53	0.41
1:B:50:LEU:C	1:B:52:PHE:N	2.74	0.41
1:B:224:GLY:O	1:B:227:VAL:HB	2.21	0.41
1:A:260:ALA:HB2	8:A:1410:PLM:HE2	2.02	0.41
1:B:64:GLN:CG	1:B:339:LYS:HE2	2.29	0.41
1:B:189:ILE:HA	1:B:189:ILE:HD13	1.94	0.41
1:B:283:PHE:HA	10:B:1506:HTG:H61	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:239:GLU:OE1	1:B:239:GLU:HA	2.20	0.41
1:A:227:VAL:O	1:A:231:LYS:HG2	2.21	0.41
1:B:140:CYS:O	1:B:141:LYS:C	2.58	0.41
1:B:27:PRO:HB3	1:B:29:TYR:CE2	2.56	0.41
1:A:72:LEU:HG	1:A:76:LEU:HD12	2.02	0.41
1:B:226:LEU:CD1	1:B:226:LEU:N	2.83	0.41
1:A:169:ALA:O	1:A:172:LEU:HB2	2.21	0.41
1:B:175:TRP:NE1	1:B:203:PHE:HB2	2.35	0.41
1:B:244:GLN:NE2	1:B:245:LYS:N	2.68	0.40
1:B:130:VAL:HG21	1:B:160:THR:HG23	2.03	0.40
1:B:158:ALA:O	1:B:162:VAL:HG23	2.21	0.40
1:B:52:PHE:C	1:B:52:PHE:CD1	2.94	0.40
1:B:125:LEU:HB2	1:B:261:PHE:CZ	2.57	0.40
1:A:232:GLU:CB	1:A:252:ARG:HD3	2.51	0.40
1:B:94:THR:HG22	1:B:113:GLU:HG3	2.00	0.40
1:B:258:VAL:O	1:B:261:PHE:HB3	2.20	0.40
1:B:332:GLU:O	1:B:333:ALA:CB	2.68	0.40
1:B:75:ILE:HG13	1:B:131:LEU:HD12	2.03	0.40
1:A:236:GLN:O	1:A:245:LYS:HD2	2.21	0.40
1:B:64:GLN:NE2	1:B:65:HIS:NE2	2.70	0.40
1:B:137:VAL:HG12	1:B:137:VAL:O	2.21	0.40

All (4) 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	Distance(Å)	Clash(Å)
1:A:279:GLN:OE1	1:B:196:GLU:OE2[2_655]	2.04	0.16
1:A:196:GLU:CD	6:B:958:ZN:ZN[2_655]	2.06	0.14
1:B:196:GLU:CD	6:A:957:ZN:ZN[2_654]	2.16	0.04
1:A:344:GLN:NE2	10:B:1509:HTG:O6[4_564]	2.19	0.01

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	347/349 (99%)	264 (76%)	57 (16%)	26 (8%)	2	3
1	B	347/349 (99%)	254 (73%)	69 (20%)	24 (7%)	2	4
All	All	694/698 (99%)	518 (75%)	126 (18%)	50 (7%)	2	4

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	SER
1	A	241	ALA
1	A	323	CYS
1	A	328	LEU
1	A	341	GLU
1	B	229	THR
1	B	240	SER
1	B	241	ALA
1	B	281	SER
1	B	331	ASP
1	B	337	VAL
1	B	341	GLU
1	B	347	PRO
1	A	195	HIS
1	A	229	THR
1	A	279	GLN
1	A	281	SER
1	A	301	TYR
1	A	324	GLY
1	A	329	GLY
1	A	335	THR
1	A	347	PRO
1	B	195	HIS
1	B	237	GLN
1	B	323	CYS
1	B	324	GLY
1	A	87	VAL
1	A	93	THR
1	A	94	THR
1	A	115	PHE
1	A	119	LEU
1	A	167	CYS
1	A	338	SER
1	B	236	GLN
1	B	238	GLN

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Mol	Chain	Res	Type
1	A	89	GLY
1	A	201	GLU
1	B	51	GLY
1	B	161	TRP
1	B	260	ALA
1	A	141	LYS
1	A	145	ASN
1	B	262	LEU
1	B	87	VAL
1	B	218	VAL
1	B	329	GLY
1	B	133	ILE
1	A	337	VAL
1	B	141	LYS
1	B	305	ILE

5.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	296/296 (100%)	276 (93%)	20 (7%)	22	54
1	B	296/296 (100%)	273 (92%)	23 (8%)	18	45
All	All	592/592 (100%)	549 (93%)	43 (7%)	20	49

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	76	LEU
1	A	78	ASN
1	A	100	HIS
1	A	119	LEU
1	A	131	LEU
1	A	135	ARG
1	A	143	MET
1	A	165	LEU
1	A	179	ILE

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Mol	Chain	Res	Type
1	A	191	TYR
1	A	237	GLN
1	A	244	GLN
1	A	245	LYS
1	A	266	LEU
1	A	302	ASN
1	A	332	GLU
1	A	336	THR
1	A	337	VAL
1	A	343	SER
1	B	8	ASN
1	B	50	LEU
1	B	70	THR
1	B	104	VAL
1	B	134	GLU
1	B	135	ARG
1	B	143	MET
1	B	148	PHE
1	B	161	TRP
1	B	185	CYS
1	B	208	PHE
1	B	220	PHE
1	B	229	THR
1	B	236	GLN
1	B	237	GLN
1	B	244	GLN
1	B	245	LYS
1	B	249	GLU
1	B	266	LEU
1	B	283	PHE
1	B	330	ASP
1	B	332	GLU
1	B	341	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	73	ASN
1	A	100	HIS
1	A	237	GLN
1	A	302	ASN

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Mol	Chain	Res	Type
1	A	312	GLN
1	A	326	ASN
1	B	8	ASN
1	B	64	GLN
1	B	73	ASN
1	B	151	ASN
1	B	237	GLN
1	B	244	GLN
1	B	302	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

11 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MAN	A	503	2	10,11,12	0.47	0	11,15,17	0.64	0
2	NAG	A	504	2	12,14,15	0.79	0	15,19,21	0.87	0
2	NAG	A	505	1,2	12,14,15	0.59	0	15,19,21	0.83	0
4	NAG	A	704	4	12,14,15	0.60	0	15,19,21	0.84	1 (6%)
4	NAG	A	705	1,4	12,14,15	0.59	0	15,19,21	0.80	1 (6%)
3	BMA	B	602	3	10,11,12	0.66	0	11,15,17	0.54	0
3	BMA	B	603	3	10,11,12	0.74	0	11,15,17	0.73	1 (9%)
3	NAG	B	604	3	12,14,15	0.58	0	15,19,21	0.95	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	605	1,3	12,14,15	0.63	0	15,19,21	0.80	1 (6%)
4	NAG	B	804	4	12,14,15	0.49	0	15,19,21	0.78	1 (6%)
4	NAG	B	805	1,4	12,14,15	0.65	0	15,19,21	0.77	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
2	MAN	A	503	2	-	0/2/19/22	0/1/1/1
2	NAG	A	504	2	-	0/6/23/26	0/1/1/1
2	NAG	A	505	1,2	-	0/6/23/26	0/1/1/1
4	NAG	A	704	4	-	0/6/23/26	0/1/1/1
4	NAG	A	705	1,4	-	0/6/23/26	0/1/1/1
3	BMA	B	602	3	-	0/2/19/22	0/1/1/1
3	BMA	B	603	3	-	0/2/19/22	0/1/1/1
3	NAG	B	604	3	-	0/6/23/26	0/1/1/1
3	NAG	B	605	1,3	-	0/6/23/26	0/1/1/1
4	NAG	B	804	4	-	0/6/23/26	0/1/1/1
4	NAG	B	805	1,4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	704	NAG	C2-N2-C7	-2.67	118.61	123.09
3	B	604	NAG	C2-N2-C7	-2.36	119.13	123.09
4	A	705	NAG	C2-N2-C7	-2.33	119.18	123.09
3	B	605	NAG	C3-C2-N2	-2.13	108.52	111.76
3	B	603	BMA	C4-C3-C2	-2.11	107.67	110.50
4	B	804	NAG	C3-C2-N2	-2.00	108.71	111.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

Of 26 ligands modelled in this entry, 13 are monoatomic - leaving 13 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$
7	RET	A	1296	1	19,20,21	2.46	3 (15%)	26,27,28	2.00	7 (26%)
8	PLM	A	1322	1	14,16,17	0.29	0	13,15,17	0.55	0
8	PLM	A	1323	1	14,16,17	0.36	0	13,15,17	0.46	0
8	PLM	A	1410	-	14,15,17	1.73	3 (21%)	13,14,17	3.26	5 (38%)
10	HTG	A	1507	-	19,19,19	3.33	8 (42%)	24,24,24	2.76	2 (8%)
10	HTG	A	1508	-	19,19,19	2.51	8 (42%)	24,24,24	3.32	3 (12%)
7	RET	B	1296	1	19,20,21	2.12	3 (15%)	26,27,28	1.88	7 (26%)
8	PLM	B	1322	1	14,16,17	0.46	0	13,15,17	0.33	0
8	PLM	B	1323	1	14,16,17	0.49	0	13,15,17	0.35	0
9	HTO	B	1401	-	9,9,9	1.63	1 (11%)	10,10,10	1.20	1 (10%)
8	PLM	B	1407	-	14,15,17	1.67	3 (21%)	13,14,17	3.24	6 (46%)
10	HTG	B	1506	-	19,19,19	3.11	8 (42%)	24,24,24	2.42	3 (12%)
10	HTG	B	1509	-	19,19,19	2.83	8 (42%)	24,24,24	2.78	3 (12%)

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
7	RET	A	1296	1	-	0/13/30/31	0/1/1/1
8	PLM	A	1322	1	-	0/13/14/15	0/0/0/0
8	PLM	A	1323	1	-	0/13/14/15	0/0/0/0
8	PLM	A	1410	-	-	0/13/13/15	0/0/0/0
10	HTG	A	1507	-	-	0/10/30/30	0/1/1/1
10	HTG	A	1508	-	-	0/10/30/30	0/1/1/1
7	RET	B	1296	1	-	0/13/30/31	0/1/1/1
8	PLM	B	1322	1	-	0/13/14/15	0/0/0/0
8	PLM	B	1323	1	-	0/13/14/15	0/0/0/0
9	HTO	B	1401	-	-	0/10/10/10	0/0/0/0
8	PLM	B	1407	-	-	0/13/13/15	0/0/0/0
10	HTG	B	1506	-	-	0/10/30/30	0/1/1/1
10	HTG	B	1509	-	-	0/10/30/30	0/1/1/1

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1507	HTG	O5-C1	9.65	1.57	1.42
10	B	1506	HTG	O5-C1	9.21	1.56	1.42
10	B	1509	HTG	O5-C1	8.19	1.54	1.42
10	A	1508	HTG	O5-C1	7.25	1.53	1.42
7	A	1296	RET	C5-C6	7.04	1.45	1.34
7	A	1296	RET	C1-C6	6.96	1.63	1.53
7	B	1296	RET	C5-C6	6.13	1.44	1.34
10	A	1507	HTG	C1-S1	5.73	1.89	1.80
7	B	1296	RET	C1-C6	5.49	1.61	1.53
10	A	1507	HTG	C1-C2	4.85	1.61	1.53
10	B	1506	HTG	C1-S1	4.70	1.87	1.80
10	B	1509	HTG	C4-C5	4.47	1.62	1.53
10	B	1509	HTG	C1-C2	4.43	1.60	1.53
8	A	1410	PLM	CC-CB	-4.42	1.24	1.51
8	B	1407	PLM	CC-CB	-4.23	1.25	1.51
10	B	1506	HTG	C3-C2	3.92	1.62	1.52
9	B	1401	HTO	C3-C2	3.74	1.63	1.52
10	B	1506	HTG	C4-C5	3.68	1.61	1.53
10	A	1507	HTG	C3-C2	3.67	1.62	1.52
10	B	1506	HTG	C1-C2	3.63	1.59	1.53
10	A	1508	HTG	C4-C5	3.62	1.61	1.53
10	A	1507	HTG	C4-C5	3.51	1.60	1.53
10	A	1507	HTG	O5-C5	3.41	1.52	1.44
10	A	1508	HTG	C1-C2	3.34	1.59	1.53
10	B	1506	HTG	O5-C5	3.32	1.52	1.44
10	B	1509	HTG	O5-C5	3.24	1.52	1.44
10	B	1506	HTG	C4-C3	3.21	1.60	1.52
10	A	1507	HTG	C4-C3	3.21	1.60	1.52
10	A	1508	HTG	O5-C5	3.14	1.52	1.44
10	B	1509	HTG	C3-C2	3.11	1.60	1.52
8	A	1410	PLM	CB-CA	-3.06	1.32	1.51
10	B	1509	HTG	C1-S1	3.04	1.85	1.80
10	B	1509	HTG	C4-C3	3.02	1.60	1.52
10	A	1508	HTG	C3-C2	3.00	1.60	1.52
10	A	1508	HTG	C4-C3	2.97	1.60	1.52
10	B	1506	HTG	C1'-S1	2.91	1.85	1.81
8	B	1407	PLM	CB-CA	-2.87	1.33	1.51
10	A	1507	HTG	C1'-S1	2.85	1.85	1.81
8	A	1410	PLM	CD-CC	-2.73	1.34	1.51
8	B	1407	PLM	CD-CC	-2.54	1.35	1.51
10	A	1508	HTG	C1-S1	2.53	1.84	1.80
7	B	1296	RET	C17-C1	2.23	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1508	HTG	C1'-S1	2.21	1.84	1.81
10	B	1509	HTG	C6-C5	2.12	1.59	1.52
7	A	1296	RET	C19-C9	2.11	1.54	1.51

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1508	HTG	C1'-S1-C1	15.23	122.30	100.19
10	B	1509	HTG	C1'-S1-C1	12.70	118.62	100.19
10	A	1507	HTG	C1'-S1-C1	12.60	118.47	100.19
10	B	1506	HTG	C1'-S1-C1	10.81	115.88	100.19
8	A	1410	PLM	CD-CC-CB	7.74	156.51	114.61
8	B	1407	PLM	CD-CC-CB	7.62	155.85	114.61
8	A	1410	PLM	CA-C9-C8	7.03	152.62	114.61
8	B	1407	PLM	CA-C9-C8	6.88	151.83	114.61
7	A	1296	RET	C18-C5-C6	5.01	130.19	124.51
7	A	1296	RET	C11-C10-C9	-4.81	120.36	127.29
7	B	1296	RET	C18-C5-C6	4.49	129.60	124.51
10	A	1508	HTG	C2-C1-S1	-3.81	106.39	110.97
7	B	1296	RET	C8-C9-C10	-3.73	113.23	118.97
7	B	1296	RET	C11-C10-C9	-3.72	121.94	127.29
7	A	1296	RET	C8-C9-C10	-3.00	114.36	118.97
7	B	1296	RET	C19-C9-C10	2.96	127.12	122.92
8	B	1407	PLM	CC-CB-CA	2.95	130.59	114.61
8	A	1410	PLM	CC-CB-CA	2.93	130.46	114.61
7	B	1296	RET	C8-C7-C6	2.73	135.37	127.32
10	A	1507	HTG	O5-C1-C2	-2.63	107.03	110.42
7	A	1296	RET	C19-C9-C10	2.59	126.59	122.92
7	A	1296	RET	C18-C5-C4	-2.49	108.77	113.34
8	B	1407	PLM	CE-CD-CC	2.36	127.40	114.61
7	B	1296	RET	C2-C1-C6	2.36	114.36	110.44
7	A	1296	RET	C8-C7-C6	2.29	134.09	127.32
8	B	1407	PLM	C5-C4-C3	2.29	127.00	114.61
8	A	1410	PLM	C5-C4-C3	2.29	126.99	114.61
10	B	1509	HTG	C2'-C1'-S1	-2.25	105.65	112.64
7	A	1296	RET	C2-C1-C6	2.22	114.13	110.44
9	B	1401	HTO	O3-C3-C4	-2.22	104.17	109.28
10	B	1506	HTG	O5-C5-C6	2.17	111.68	106.34
10	B	1506	HTG	O5-C1-C2	-2.15	107.65	110.42
10	A	1508	HTG	O5-C5-C6	2.11	111.52	106.34
8	A	1410	PLM	CE-CD-CC	2.08	125.86	114.61
7	B	1296	RET	C18-C5-C4	-2.04	109.60	113.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	1509	HTG	O5-C5-C6	2.03	111.32	106.34
8	B	1407	PLM	C9-C8-C7	2.01	125.50	114.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	349/349 (100%)	2.16	200 (57%)  	48, 61, 135, 149	228 (65%)
1	B	349/349 (100%)	2.41	222 (63%)  	48, 64, 154, 163	228 (65%)
All	All	698/698 (100%)	2.28	422 (60%)  	48, 63, 147, 163	456 (65%)

All (422) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	348	ALA	10.8
1	B	232	GLU	10.4
1	B	142	PRO	9.3
1	B	148	PHE	8.0
1	B	107	PRO	7.5
1	B	163	MET	7.2
1	B	233	ALA	7.0
1	B	234	ALA	6.9
1	B	235	ALA	6.7
1	A	142	PRO	6.7
1	B	200	ASN	6.7
1	B	344	GLN	6.5
1	A	243	THR	6.1
1	B	116	PHE	6.1
1	A	295	ALA	6.1
1	B	143	MET	6.1
1	A	235	ALA	6.1
1	A	118	THR	6.1
1	A	60	TYR	6.0
1	B	321	LEU	6.0
1	A	146	PHE	6.0
1	B	296	LYS	5.9
1	B	342	THR	5.8
1	B	281	SER	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	328	LEU	5.8
1	A	294	PHE	5.7
1	B	242	THR	5.7
1	B	199	ASN	5.4
1	A	198	THR	5.4
1	A	86	MET	5.4
1	B	68	LEU	5.3
1	A	348	ALA	5.3
1	B	286	ILE	5.2
1	A	224	GLY	5.1
1	A	228	PHE	5.1
1	B	145	ASN	5.1
1	A	147	ARG	5.1
1	B	295	ALA	5.0
1	A	126	TRP	5.0
1	B	339	LYS	5.0
1	A	104	VAL	4.8
1	A	105	PHE	4.8
1	B	140	CYS	4.8
1	B	314	ARG	4.8
1	A	252	ARG	4.7
1	A	314	ARG	4.7
1	A	71	PRO	4.7
1	A	250	VAL	4.6
1	A	159	PHE	4.6
1	B	164	ALA	4.6
1	A	167	CYS	4.5
1	A	132	ALA	4.5
1	A	23	PRO	4.5
1	B	257	MET	4.4
1	B	106	GLY	4.3
1	B	322	CYS	4.3
1	B	251	THR	4.2
1	A	197	GLU	4.2
1	B	231	LYS	4.2
1	B	144	SER	4.2
1	A	333	ALA	4.1
1	A	234	ALA	4.1
1	A	176	SER	4.1
1	B	263	ILE	4.1
1	B	118	THR	4.1
1	B	84	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	96	TYR	4.0
1	A	233	ALA	4.0
1	A	145	ASN	4.0
1	A	310	ASN	4.0
1	B	87	VAL	3.9
1	A	265	TRP	3.9
1	B	185	CYS	3.9
1	A	242	THR	3.9
1	B	104	VAL	3.9
1	B	43	TYR	3.9
1	B	291	PRO	3.9
1	A	100	HIS	3.9
1	A	190	ASP	3.9
1	B	265	TRP	3.9
1	A	64	GLN	3.9
1	A	90	GLY	3.9
1	B	182	GLY	3.9
1	A	130	VAL	3.9
1	B	228	PHE	3.8
1	B	340	THR	3.8
1	B	230	VAL	3.8
1	B	99	LEU	3.8
1	A	97	THR	3.8
1	A	80	ALA	3.7
1	A	75	ILE	3.7
1	B	332	GLU	3.7
1	B	311	LYS	3.7
1	B	115	PHE	3.7
1	B	229	THR	3.7
1	B	74	TYR	3.7
1	B	256	ILE	3.6
1	A	298	SER	3.6
1	A	39	MET	3.6
1	B	179	ILE	3.6
1	A	240	SER	3.6
1	A	307	ILE	3.6
1	B	262	LEU	3.6
1	A	236	GLN	3.5
1	B	62	THR	3.5
1	B	167	CYS	3.5
1	B	329	GLY	3.5
1	B	258	VAL	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	215	PRO	3.5
1	B	168	ALA	3.5
1	B	131	LEU	3.5
1	A	47	LEU	3.5
1	B	162	VAL	3.5
1	B	275	ILE	3.5
1	A	33	GLU	3.5
1	B	273	PHE	3.5
1	B	89	GLY	3.4
1	A	113	GLU	3.4
1	A	315	ASN	3.4
1	B	47	LEU	3.4
1	B	19	VAL	3.4
1	A	32	ALA	3.4
1	A	283	PHE	3.4
1	A	306	TYR	3.4
1	A	185	CYS	3.4
1	A	304	VAL	3.4
1	B	254	VAL	3.4
1	B	206	TYR	3.4
1	B	220	PHE	3.4
1	A	125	LEU	3.4
1	A	189	ILE	3.4
1	A	291	PRO	3.3
1	B	210	VAL	3.3
1	B	198	THR	3.3
1	B	86	MET	3.3
1	A	76	LEU	3.3
1	A	88	PHE	3.3
1	B	125	LEU	3.3
1	A	269	ALA	3.2
1	B	345	VAL	3.2
1	B	79	LEU	3.2
1	A	302	ASN	3.2
1	A	16	LYS	3.2
1	A	305	ILE	3.2
1	B	208	PHE	3.2
1	B	165	LEU	3.2
1	B	207	MET	3.2
1	B	114	GLY	3.2
1	B	253	MET	3.2
1	B	60	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	236	GLN	3.2
1	B	103	PHE	3.2
1	A	163	MET	3.1
1	B	173	VAL	3.1
1	B	287	PHE	3.1
1	B	298	SER	3.1
1	B	308	MET	3.1
1	A	166	ALA	3.1
1	B	271	VAL	3.1
1	A	282	ASP	3.1
1	A	214	ILE	3.1
1	B	269	ALA	3.1
1	A	120	GLY	3.1
1	A	148	PHE	3.1
1	B	159	PHE	3.1
1	B	294	PHE	3.1
1	B	176	SER	3.1
1	A	267	PRO	3.1
1	A	131	LEU	3.0
1	A	43	TYR	3.0
1	B	105	PHE	3.0
1	B	161	TRP	3.0
1	A	58	THR	3.0
1	B	285	PRO	3.0
1	A	309	MET	3.0
1	A	84	LEU	3.0
1	A	313	PHE	3.0
1	A	281	SER	3.0
1	A	41	ALA	3.0
1	A	218	VAL	3.0
1	B	146	PHE	3.0
1	B	240	SER	3.0
1	A	204	VAL	3.0
1	B	158	ALA	3.0
1	B	64	GLN	3.0
1	B	55	ASN	3.0
1	A	292	ALA	3.0
1	B	96	TYR	3.0
1	B	56	PHE	3.0
1	A	217	ILE	2.9
1	A	316	CYS	2.9
1	B	172	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	276	PHE	2.9
1	A	161	TRP	2.9
1	B	108	THR	2.9
1	A	287	PHE	2.9
1	B	171	PRO	2.9
1	A	303	PRO	2.9
1	A	35	TRP	2.9
1	A	42	ALA	2.9
1	B	191	TYR	2.9
1	A	192	TYR	2.8
1	A	272	ALA	2.8
1	A	128	LEU	2.8
1	A	155	MET	2.8
1	B	272	ALA	2.8
1	B	289	THR	2.8
1	B	313	PHE	2.8
1	A	94	THR	2.8
1	B	94	THR	2.8
1	B	243	THR	2.8
1	A	44	MET	2.8
1	B	98	SER	2.8
1	B	38	SER	2.8
1	B	267	PRO	2.8
1	A	74	TYR	2.8
1	A	266	LEU	2.8
1	B	212	PHE	2.8
1	A	337	VAL	2.8
1	B	334	SER	2.8
1	A	121	GLY	2.8
1	B	218	VAL	2.8
1	B	303	PRO	2.8
1	B	21	ARG	2.7
1	A	209	VAL	2.7
1	A	327	PRO	2.7
1	A	77	LEU	2.7
1	B	261	PHE	2.7
1	A	200	ASN	2.7
1	B	297	THR	2.7
1	A	119	LEU	2.7
1	B	65	HIS	2.7
1	B	238	GLN	2.7
1	B	187	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	80	ALA	2.7
1	B	126	TRP	2.7
1	B	343	SER	2.7
1	B	124	ALA	2.7
1	B	211	HIS	2.7
1	B	277	THR	2.7
1	A	179	ILE	2.7
1	B	284	GLY	2.7
1	B	44	MET	2.7
1	A	127	SER	2.7
1	B	266	LEU	2.7
1	A	301	TYR	2.7
1	B	330	ASP	2.7
1	B	264	CYS	2.7
1	A	95	LEU	2.7
1	A	115	PHE	2.7
1	A	300	VAL	2.6
1	B	219	ILE	2.6
1	B	53	PRO	2.6
1	A	48	ILE	2.6
1	B	81	VAL	2.6
1	A	212	PHE	2.6
1	A	171	PRO	2.6
1	B	82	ALA	2.6
1	A	199	ASN	2.6
1	B	78	ASN	2.6
1	B	127	SER	2.6
1	B	186	SER	2.6
1	A	206	TYR	2.6
1	B	117	ALA	2.6
1	A	110	CYS	2.6
1	A	91	PHE	2.6
1	B	283	PHE	2.6
1	A	297	THR	2.6
1	A	49	MET	2.6
1	A	65	HIS	2.6
1	B	175	TRP	2.6
1	B	336	THR	2.6
1	A	143	MET	2.6
1	B	178	TYR	2.6
1	A	271	VAL	2.6
1	B	91	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	189	ILE	2.6
1	B	58	THR	2.6
1	B	260	ALA	2.6
1	B	288	MET	2.5
1	B	300	VAL	2.5
1	A	170	PRO	2.5
1	A	178	TYR	2.5
1	A	45	PHE	2.5
1	B	290	ILE	2.5
1	A	254	VAL	2.5
1	A	284	GLY	2.5
1	A	46	LEU	2.5
1	A	241	ALA	2.5
1	B	309	MET	2.5
1	A	160	THR	2.5
1	A	81	VAL	2.5
1	B	157	VAL	2.5
1	B	153	ALA	2.5
1	B	83	ASP	2.5
1	A	72	LEU	2.5
1	A	247	GLU	2.5
1	B	201	GLU	2.5
1	B	241	ALA	2.5
1	A	251	THR	2.5
1	B	160	THR	2.5
1	B	307	ILE	2.5
1	B	36	GLN	2.5
1	A	102	TYR	2.5
1	A	220	PHE	2.5
1	A	188	GLY	2.5
1	A	98	SER	2.5
1	A	216	LEU	2.5
1	B	239	GLU	2.4
1	B	217	ILE	2.4
1	B	225	GLN	2.4
1	B	305	ILE	2.4
1	B	73	ASN	2.4
1	B	147	ARG	2.4
1	A	196	GLU	2.4
1	B	76	LEU	2.4
1	B	320	THR	2.4
1	A	182	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	82	ALA	2.4
1	A	260	ALA	2.4
1	A	183	MET	2.4
1	A	275	ILE	2.4
1	A	78	ASN	2.4
1	B	274	TYR	2.4
1	B	306	TYR	2.4
1	B	95	LEU	2.3
1	B	119	LEU	2.3
1	B	203	PHE	2.3
1	B	197	GLU	2.3
1	A	211	HIS	2.3
1	A	168	ALA	2.3
1	B	292	ALA	2.3
1	A	268	TYR	2.3
1	A	55	ASN	2.3
1	B	310	ASN	2.3
1	B	174	GLY	2.3
1	B	54	ILE	2.3
1	A	87	VAL	2.3
1	B	214	ILE	2.3
1	A	237	GLN	2.3
1	B	130	VAL	2.3
1	A	54	ILE	2.3
1	B	71	PRO	2.3
1	A	193	THR	2.3
1	A	124	ALA	2.3
1	A	210	VAL	2.3
1	B	293	PHE	2.3
1	A	334	SER	2.3
1	A	276	PHE	2.3
1	A	205	ILE	2.3
1	B	46	LEU	2.3
1	B	50	LEU	2.3
1	B	72	LEU	2.3
1	B	128	LEU	2.3
1	A	14	SER	2.3
1	A	38	SER	2.3
1	A	280	GLY	2.3
1	B	188	GLY	2.3
1	B	301	TYR	2.3
1	B	304	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	232	GLU	2.2
1	A	40	LEU	2.2
1	A	79	LEU	2.2
1	B	209	VAL	2.2
1	B	97	THR	2.2
1	B	252	ARG	2.2
1	A	111	ASN	2.2
1	A	123	ILE	2.2
1	A	195	HIS	2.2
1	A	117	ALA	2.2
1	B	88	PHE	2.2
1	A	263	ILE	2.2
1	B	75	ILE	2.2
1	A	270	GLY	2.2
1	A	164	ALA	2.2
1	B	302	ASN	2.2
1	A	213	ILE	2.2
1	B	51	GLY	2.2
1	A	296	LYS	2.2
1	A	175	TRP	2.2
1	B	183	MET	2.2
1	B	194	PRO	2.2
1	A	53	PRO	2.1
1	B	331	ASP	2.1
1	B	52	PHE	2.1
1	B	312	GLN	2.1
1	A	158	ALA	2.1
1	A	17	THR	2.1
1	A	277	THR	2.1
1	B	341	GLU	2.1
1	A	156	GLY	2.1
1	B	282	ASP	2.1
1	A	191	TYR	2.1
1	A	59	LEU	2.1
1	B	90	GLY	2.1
1	A	70	THR	2.1
1	A	51	GLY	2.1
1	B	204	VAL	2.1
1	B	166	ALA	2.1
1	B	102	TYR	2.1
1	A	273	PHE	2.1
1	A	202	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	40	LEU	2.1
1	A	194	PRO	2.1
1	B	61	VAL	2.1
1	B	137	VAL	2.1
1	B	213	ILE	2.1
1	A	308	MET	2.1
1	A	285	PRO	2.0
1	A	129	VAL	2.0
1	B	42	ALA	2.0
1	A	57	LEU	2.0
1	A	109	GLY	2.0
1	A	61	VAL	2.0
1	A	258	VAL	2.0
1	B	255	ILE	2.0
1	A	262	LEU	2.0
1	A	278	HIS	2.0
1	B	259	ILE	2.0
1	B	26	ALA	2.0
1	B	101	GLY	2.0
1	B	121	GLY	2.0

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 ⓘ

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
4	NAG	B	805	14/15	0.26	-0.18	65,69,71,77	0
3	BMA	B	602	11/12	0.33	-0.29	120,122,122,124	0
3	NAG	B	605	14/15	0.19	-0.60	63,64,69,75	0
3	NAG	B	604	14/15	0.23	-0.85	77,83,90,97	0
2	NAG	A	505	14/15	0.16	-0.97	66,68,74,75	0
2	NAG	A	504	14/15	0.22	-1.11	79,82,87,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	A	705	14/15	0.18	-1.33	70,75,80,84	0
3	BMA	B	603	11/12	0.25	-1.71	104,108,112,116	0
4	NAG	B	804	14/15	0.28	-	84,89,91,92	0
4	NAG	A	704	14/15	0.28	-	91,94,99,101	0
2	MAN	A	503	11/12	0.22	-	94,97,97,99	0

6.4 Ligands

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(\AA^2)	Q<0.9
7	RET	A	1296	20/21	0.71	4.16	50,52,54,55	20
8	PLM	A	1322	17/18	0.49	2.68	94,104,110,110	0
8	PLM	B	1407	16/18	0.50	2.36	75,82,87,88	0
7	RET	B	1296	20/21	0.51	1.15	51,52,54,54	20
8	PLM	B	1323	17/18	0.45	0.59	117,122,124,124	0
8	PLM	B	1322	17/18	0.44	0.46	105,108,109,110	0
10	HTG	B	1509	19/19	0.40	0.06	93,95,100,100	0
10	HTG	A	1507	19/19	0.39	-0.04	99,113,115,116	0
6	ZN	B	963	1/1	0.43	-0.14	93,93,93,93	1
5	HG	A	905	1/1	0.34	-0.14	99,99,99,99	1
8	PLM	A	1323	17/18	0.28	-0.24	98,105,113,114	0
5	HG	B	906	1/1	0.23	-0.60	121,121,121,121	1
10	HTG	A	1508	19/19	0.23	-0.83	72,78,82,85	0
6	ZN	A	962	1/1	0.32	-0.99	80,80,80,80	1
10	HTG	B	1506	19/19	0.33	-1.10	88,93,97,99	0
5	HG	A	903	1/1	0.12	-1.38	96,96,96,96	1
5	HG	B	904	1/1	0.13	-1.42	109,109,109,109	1
6	ZN	A	2011	1/1	0.04	-1.96	53,53,53,53	1
8	PLM	A	1410	16/18	0.29	-2.20	74,77,79,79	0
9	HTO	B	1401	10/10	0.20	-2.23	56,60,62,63	0
6	ZN	B	956	1/1	0.08	-2.71	60,60,60,60	1
5	HG	A	901	1/1	0.08	-2.73	82,82,82,82	1
6	ZN	A	957	1/1	0.07	-2.76	53,53,53,53	1
6	ZN	A	959	1/1	0.07	-2.98	92,92,92,92	1
6	ZN	B	958	1/1	0.15	-5.39	43,43,43,43	1
5	HG	B	902	1/1	0.05	-5.51	80,80,80,80	1

6.5 Other polymers ⓘ

There are no such residues in this entry.