



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:23 PM UTC

PDB ID : 3CSN / pdb_00003csn
Title : Structure of the Serratia marcescens hemophore receptor HasR in complex with its hemophore HasA
Authors : Krieg, S.; Diederichs, K.
Deposited on : 2008-04-10
Resolution : 3.00 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

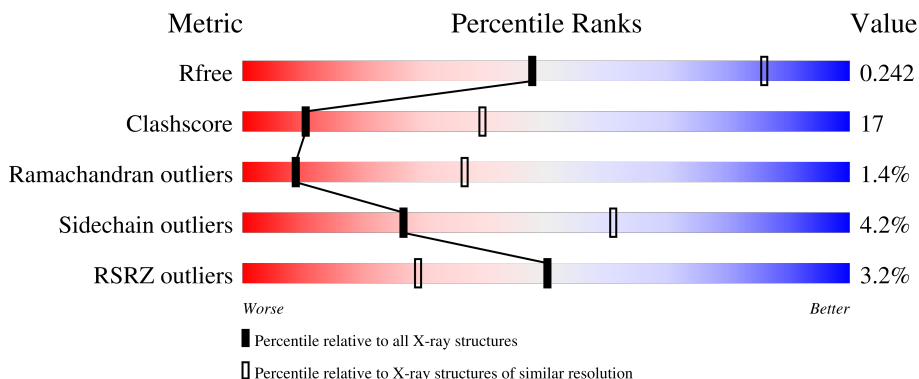
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	865	
1	B	865	
2	C	206	
2	D	206	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14195 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 HasR protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	753	Total	C	N	O	S	0	0	0
			5889	3674	1043	1159	13			
1	B	753	Total	C	N	O	S	0	0	0
			5889	3674	1043	1159	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	645	ALA	GLY	SEE REMARK 999	UNP Q79AD2
B	645	ALA	GLY	SEE REMARK 999	UNP Q79AD2

- Molecule 2 is a protein called Hemophore HasA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	163	Total	C	N	O	S	0	0	0
			1184	743	189	251	1			
2	D	163	Total	C	N	O	S	0	0	0
			1184	743	189	251	1			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	MET	-	expression tag	UNP Q54450
C	-16	ARG	-	expression tag	UNP Q54450
C	-15	GLY	-	expression tag	UNP Q54450
C	-14	SER	-	expression tag	UNP Q54450
C	-13	HIS	-	expression tag	UNP Q54450
C	-12	HIS	-	expression tag	UNP Q54450
C	-11	HIS	-	expression tag	UNP Q54450
C	-10	HIS	-	expression tag	UNP Q54450
C	-9	HIS	-	expression tag	UNP Q54450
C	-8	HIS	-	expression tag	UNP Q54450

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-7	GLY	-	expression tag	UNP Q54450
C	-6	ILE	-	expression tag	UNP Q54450
C	-5	ARG	-	expression tag	UNP Q54450
C	-4	MET	-	expression tag	UNP Q54450
C	-3	ARG	-	expression tag	UNP Q54450
C	-2	ALA	-	expression tag	UNP Q54450
C	-1	ARG	-	expression tag	UNP Q54450
C	0	TYR	-	expression tag	UNP Q54450
C	1	PRO	-	expression tag	UNP Q54450
D	-17	MET	-	expression tag	UNP Q54450
D	-16	ARG	-	expression tag	UNP Q54450
D	-15	GLY	-	expression tag	UNP Q54450
D	-14	SER	-	expression tag	UNP Q54450
D	-13	HIS	-	expression tag	UNP Q54450
D	-12	HIS	-	expression tag	UNP Q54450
D	-11	HIS	-	expression tag	UNP Q54450
D	-10	HIS	-	expression tag	UNP Q54450
D	-9	HIS	-	expression tag	UNP Q54450
D	-8	HIS	-	expression tag	UNP Q54450
D	-7	GLY	-	expression tag	UNP Q54450
D	-6	ILE	-	expression tag	UNP Q54450
D	-5	ARG	-	expression tag	UNP Q54450
D	-4	MET	-	expression tag	UNP Q54450
D	-3	ARG	-	expression tag	UNP Q54450
D	-2	ALA	-	expression tag	UNP Q54450
D	-1	ARG	-	expression tag	UNP Q54450
D	0	TYR	-	expression tag	UNP Q54450
D	1	PRO	-	expression tag	UNP Q54450

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

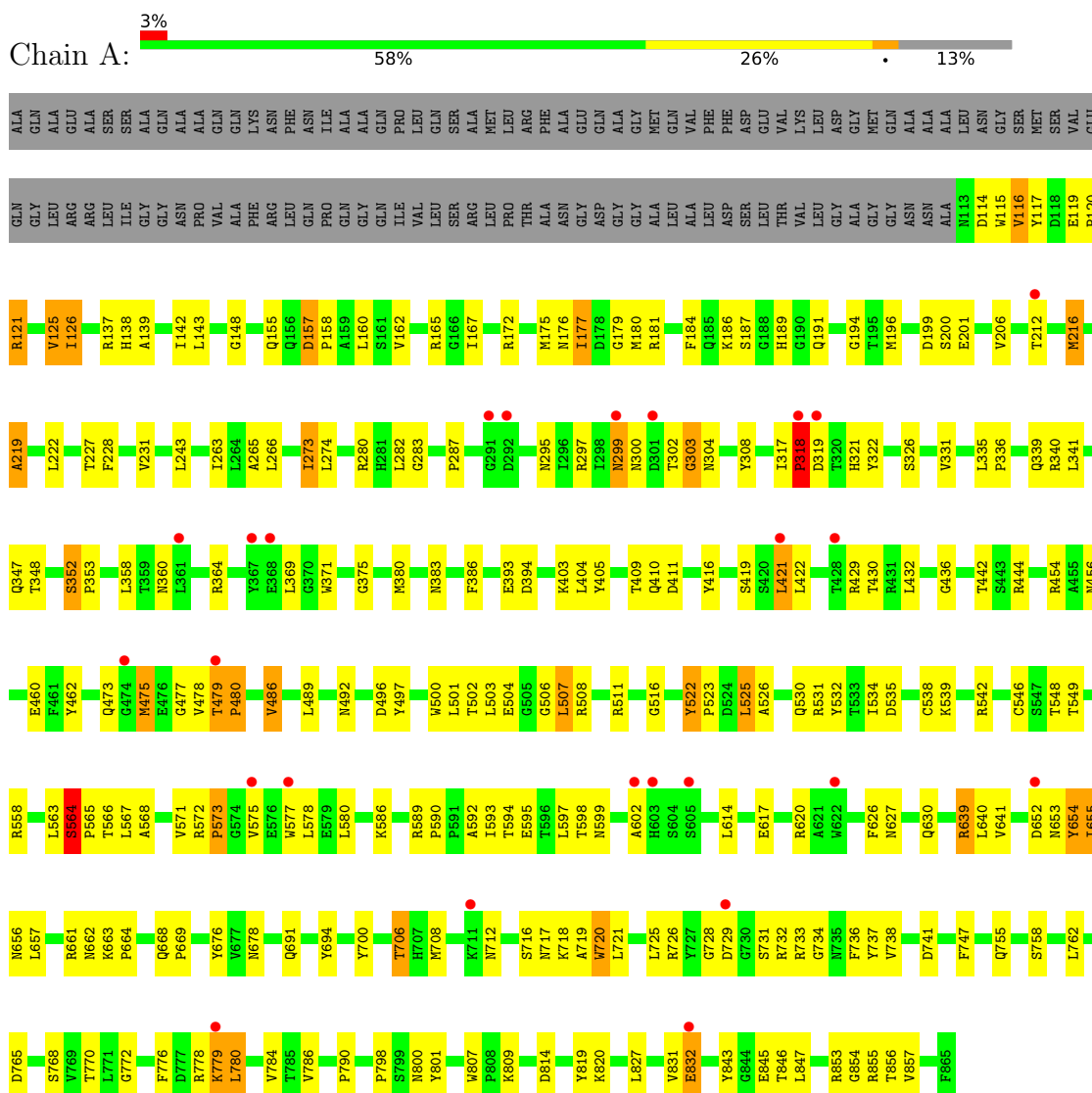
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	7	Total	O	0	0
			7	7		
4	C	1	Total	O	0	0
			1	1		
4	D	1	Total	O	0	0
			1	1		

3 Residue-property plots

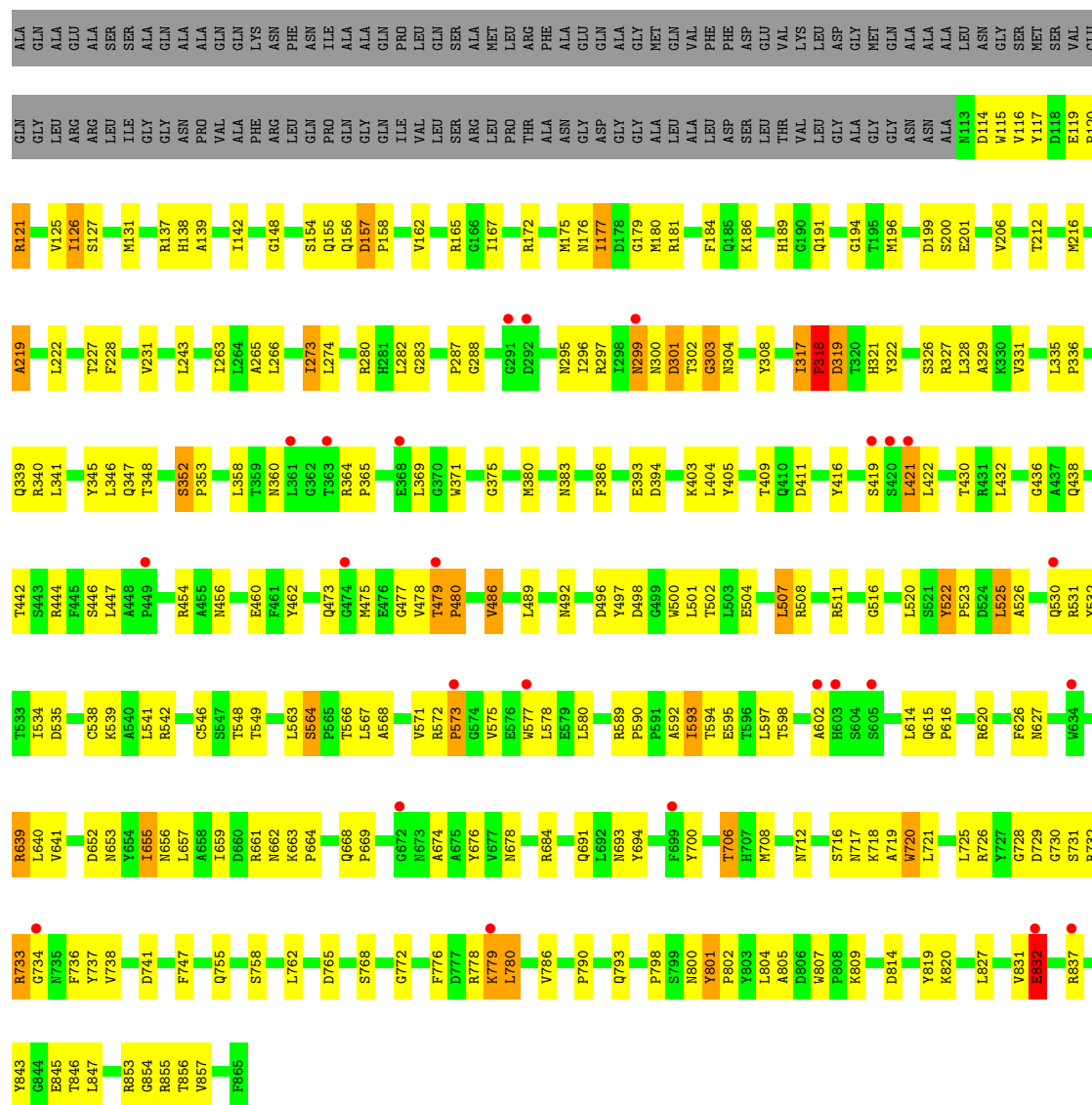
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: HasR protein

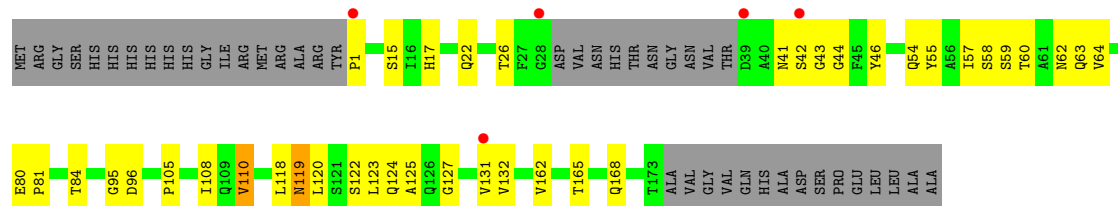


• Molecule 1: HasR protein





• Molecule 2: Hemophore HasA



• Molecule 2: Hemophore HasA





4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	157.65Å 164.74Å 597.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.43 – 3.00 49.43 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (49.43-3.00) 99.3 (49.43-3.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 3.01Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.217 , 0.244 0.215 , 0.242	Depositor DCC
R_{free} test set	3890 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	62.4	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 66.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.039 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14195	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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: 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	A	0.63	0/6027	0.93	12/8188 (0.1%)
1	B	0.63	0/6027	0.93	16/8188 (0.2%)
2	C	0.53	1/1211 (0.1%)	0.84	2/1649 (0.1%)
2	D	0.54	1/1211 (0.1%)	0.88	4/1649 (0.2%)
All	All	0.62	2/14476 (0.0%)	0.92	34/19674 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	42	SER	C-N	6.89	1.41	1.33
2	D	42	SER	C-N	5.76	1.40	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	42	SER	CA-C-N	-11.60	112.11	122.43
2	D	42	SER	C-N-CA	-11.60	112.11	122.43
2	C	42	SER	CA-C-N	-9.09	113.24	122.69
2	C	42	SER	C-N-CA	-9.09	113.24	122.69
1	A	564	SER	CA-C-N	8.64	128.58	119.85
1	A	564	SER	C-N-CA	8.64	128.58	119.85
1	B	564	SER	CA-C-N	8.48	128.41	119.85
1	B	564	SER	C-N-CA	8.48	128.41	119.85
1	B	201	GLU	N-CA-C	-7.75	104.05	113.97
1	A	201	GLU	N-CA-C	-7.57	104.28	113.97
1	B	779	LYS	N-CA-C	6.36	118.99	108.49
1	B	352	SER	CA-C-N	6.02	125.78	119.76
1	B	352	SER	C-N-CA	6.02	125.78	119.76
1	B	319	ASP	N-CA-C	-5.89	103.38	110.44
1	A	352	SER	CA-C-N	5.62	125.55	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	SER	C-N-CA	5.62	125.55	119.76
1	B	157	ASP	CA-C-N	5.61	125.70	119.87
1	B	157	ASP	C-N-CA	5.61	125.70	119.87
1	A	779	LYS	N-CA-C	5.60	117.72	108.49
1	A	318	PRO	N-CA-C	5.55	123.90	112.47
1	B	318	PRO	N-CA-C	5.52	123.83	112.47
2	D	110	VAL	CA-C-N	5.34	125.26	119.76
2	D	110	VAL	C-N-CA	5.34	125.26	119.76
1	B	684	ARG	N-CA-C	5.33	118.17	109.59
1	A	475	MET	N-CA-C	-5.24	108.65	114.62
1	B	317	ILE	N-CA-C	-5.13	104.22	108.63
1	A	522	TYR	CA-C-N	5.10	126.22	119.84
1	A	522	TYR	C-N-CA	5.10	126.22	119.84
1	B	801	TYR	CA-C-N	5.09	124.58	119.19
1	B	801	TYR	C-N-CA	5.09	124.58	119.19
1	A	157	ASP	CA-C-N	5.06	125.14	119.87
1	A	157	ASP	C-N-CA	5.06	125.14	119.87
1	B	522	TYR	CA-C-N	5.00	126.09	119.84
1	B	522	TYR	C-N-CA	5.00	126.09	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5889	0	5597	204	0
1	B	5889	0	5597	209	0
2	C	1184	0	1078	31	0
2	D	1184	0	1078	34	0
3	A	6	0	8	2	0
3	B	24	0	32	1	0
4	A	10	0	0	0	0
4	B	7	0	0	1	0
4	C	1	0	0	0	0
4	D	1	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	14195	0	13390	468	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 17.

All (468) 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)
1:A:779:LYS:HZ3	1:A:820:LYS:HG3	1.26	0.99
1:B:779:LYS:HZ3	1:B:820:LYS:HG3	1.33	0.94
1:A:575:VAL:HG22	1:A:577:TRP:H	1.35	0.91
1:B:720:TRP:CD1	1:B:721:LEU:HD13	2.08	0.88
1:B:575:VAL:HG22	1:B:577:TRP:H	1.37	0.87
1:A:720:TRP:CD1	1:A:721:LEU:HD13	2.10	0.86
1:B:162:VAL:HG23	1:B:175:MET:HE3	1.57	0.86
1:A:548:THR:HG22	1:A:549:THR:H	1.42	0.85
1:B:548:THR:HG22	1:B:549:THR:H	1.42	0.83
1:A:165:ARG:HA	1:A:708:MET:HE1	1.60	0.83
1:A:180:MET:HE1	1:A:383:ASN:HB3	1.61	0.83
1:A:216:MET:HE2	1:A:460:GLU:HB2	1.61	0.82
1:A:162:VAL:HG23	1:A:175:MET:HE3	1.60	0.82
1:B:165:ARG:HA	1:B:708:MET:HE1	1.61	0.81
1:B:526:ALA:HB2	1:B:531:ARG:HA	1.62	0.81
1:A:526:ALA:HB2	1:A:531:ARG:HA	1.64	0.80
1:B:180:MET:HE1	1:B:383:ASN:HB3	1.64	0.80
1:B:526:ALA:HB1	1:B:530:GLN:O	1.83	0.78
1:B:172:ARG:NH1	1:B:655:ILE:HD13	1.99	0.77
1:B:548:THR:HG22	1:B:549:THR:N	1.98	0.77
1:B:216:MET:HE2	1:B:460:GLU:HB2	1.66	0.77
1:B:814:ASP:OD1	1:B:832:GLU:O	2.02	0.76
1:A:548:THR:HG22	1:A:549:THR:N	2.01	0.75
1:B:593:ILE:HD12	1:B:593:ILE:H	1.50	0.75
1:A:853:ARG:HH11	1:A:856:THR:HG21	1.51	0.74
1:A:620:ARG:C	1:A:620:ARG:HD2	2.13	0.73
1:A:172:ARG:NH1	1:A:655:ILE:HD13	2.04	0.73
1:A:593:ILE:H	1:A:593:ILE:HD12	1.52	0.73
1:B:364:ARG:HD2	1:B:364:ARG:O	1.87	0.73
1:A:199:ASP:O	1:A:200:SER:HB3	1.89	0.72
1:B:318:PRO:HG2	1:B:371:TRP:HB2	1.72	0.72
1:A:364:ARG:HD2	1:A:364:ARG:O	1.90	0.71
1:B:620:ARG:HD2	1:B:620:ARG:C	2.16	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:176:ASN:ND2	1:B:179:GLY:HA2	2.05	0.71
1:A:526:ALA:HB1	1:A:530:GLN:O	1.89	0.71
1:B:199:ASP:O	1:B:200:SER:HB3	1.91	0.71
1:B:592:ALA:HB3	1:B:595:GLU:HG2	1.71	0.71
1:B:480:PRO:HG2	1:B:597:LEU:HB2	1.73	0.70
1:B:668:GLN:HG3	2:D:58:SER:HB3	1.74	0.70
1:A:731:SER:OG	1:A:733:ARG:HG2	1.93	0.69
1:B:731:SER:OG	1:B:733:ARG:HG2	1.93	0.69
1:A:318:PRO:HG2	1:A:371:TRP:HB2	1.74	0.69
1:B:827:LEU:HD23	1:B:827:LEU:H	1.58	0.69
2:C:123:LEU:H	2:C:123:LEU:HD23	1.58	0.69
1:A:827:LEU:HD23	1:A:827:LEU:H	1.57	0.69
1:A:592:ALA:HB3	1:A:595:GLU:HG2	1.75	0.68
1:A:176:ASN:ND2	1:A:179:GLY:HA2	2.07	0.68
1:B:652:ASP:O	1:B:653:ASN:HB2	1.93	0.68
1:A:639:ARG:HD2	1:A:639:ARG:C	2.19	0.67
1:B:639:ARG:C	1:B:639:ARG:HD2	2.20	0.67
1:B:300:ASN:O	1:B:302:THR:HG23	1.94	0.67
1:A:137:ARG:HD3	1:A:853:ARG:HD2	1.77	0.66
1:A:798:PRO:HB2	1:A:800:ASN:OD1	1.95	0.66
1:A:814:ASP:OD1	1:A:832:GLU:O	2.13	0.66
1:B:589:ARG:HH12	1:B:655:ILE:HD12	1.60	0.66
1:B:526:ALA:CB	1:B:531:ARG:HA	2.25	0.66
2:D:123:LEU:HD23	2:D:123:LEU:H	1.60	0.66
1:B:798:PRO:HB2	1:B:800:ASN:OD1	1.95	0.66
1:B:853:ARG:HH11	1:B:856:THR:HG21	1.59	0.66
1:A:480:PRO:HG2	1:A:597:LEU:HB2	1.75	0.66
1:B:778:ARG:O	1:B:778:ARG:HG3	1.96	0.65
1:A:526:ALA:CB	1:A:531:ARG:HA	2.26	0.65
1:A:177:ILE:HG22	1:A:228:PHE:HB2	1.79	0.65
2:C:124:GLN:O	2:C:125:ALA:HB3	1.96	0.65
1:A:668:GLN:HG3	2:C:58:SER:HB3	1.78	0.64
1:A:539:LYS:HA	1:A:734:GLY:HA2	1.80	0.64
1:A:589:ARG:HH12	1:A:655:ILE:HD12	1.63	0.64
1:B:177:ILE:HG22	1:B:228:PHE:HB2	1.80	0.64
1:A:283:GLY:HA2	1:A:321:HIS:HB3	1.80	0.63
1:B:539:LYS:HA	1:B:734:GLY:HA2	1.79	0.63
1:A:475:MET:HA	1:A:478:VAL:HG23	1.79	0.63
1:A:180:MET:CE	1:A:383:ASN:HB3	2.29	0.63
1:B:180:MET:CE	1:B:383:ASN:HB3	2.28	0.63
1:A:652:ASP:O	1:A:653:ASN:HB2	1.97	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:17:HIS:HB2	2:D:162:VAL:HG22	1.82	0.62
1:A:326:SER:HB3	1:A:348:THR:HB	1.81	0.62
1:A:216:MET:CE	1:A:460:GLU:HB2	2.30	0.61
1:A:548:THR:CG2	1:A:549:THR:H	2.13	0.61
1:A:480:PRO:HG3	1:A:598:THR:HA	1.82	0.61
1:A:589:ARG:HH12	1:A:655:ILE:CD1	2.14	0.61
1:A:798:PRO:HD2	1:A:801:TYR:CE1	2.36	0.61
2:D:124:GLN:O	2:D:125:ALA:HB3	2.00	0.61
1:B:548:THR:CG2	1:B:549:THR:H	2.14	0.61
1:B:589:ARG:HH12	1:B:655:ILE:CD1	2.14	0.61
1:A:779:LYS:HG2	1:A:820:LYS:HB2	1.83	0.60
1:A:335:LEU:HB3	1:A:336:PRO:HD2	1.83	0.60
1:A:297:ARG:HH22	1:A:847:LEU:HA	1.66	0.60
1:A:669:PRO:HB3	2:C:44:GLY:HA3	1.82	0.60
2:D:122:SER:HB2	2:D:132:VAL:HG23	1.83	0.60
2:D:96:ASP:HB2	2:D:110:VAL:HG13	1.84	0.59
2:D:46:TYR:HB3	2:D:54:GLN:HG2	1.84	0.59
1:B:137:ARG:HD3	1:B:853:ARG:HD2	1.85	0.59
1:B:283:GLY:HA2	1:B:321:HIS:HB3	1.84	0.59
2:D:165:THR:OG1	2:D:168:GLN:HG3	2.02	0.59
2:C:96:ASP:HB2	2:C:110:VAL:HG13	1.84	0.59
1:B:297:ARG:HH22	1:B:847:LEU:HA	1.67	0.59
1:A:283:GLY:HA2	1:A:321:HIS:CB	2.33	0.59
1:B:216:MET:CE	1:B:460:GLU:HB2	2.33	0.58
1:B:726:ARG:HB2	1:B:741:ASP:HB2	1.84	0.58
1:B:335:LEU:HB3	1:B:336:PRO:HD2	1.85	0.58
1:A:403:LYS:C	1:A:404:LEU:HD12	2.28	0.58
1:B:730:GLY:HA3	4:B:873:HOH:O	2.02	0.58
1:A:779:LYS:HG2	1:A:820:LYS:HZ3	1.69	0.57
2:C:17:HIS:HB2	2:C:162:VAL:HG22	1.85	0.57
1:A:765:ASP:O	1:A:790:PRO:HD2	2.03	0.57
1:B:326:SER:HB3	1:B:348:THR:HB	1.86	0.57
2:C:43:GLY:HA3	2:C:55:TYR:CZ	2.39	0.57
1:A:184:PHE:HA	1:A:432:LEU:HD23	1.86	0.57
1:A:726:ARG:HB2	1:A:741:ASP:HB2	1.84	0.57
1:B:360:ASN:ND2	2:D:81:PRO:HA	2.19	0.57
1:B:507:LEU:O	1:B:507:LEU:HD12	2.05	0.57
2:D:43:GLY:HA3	2:D:55:TYR:CZ	2.39	0.57
1:B:403:LYS:C	1:B:404:LEU:HD12	2.30	0.57
1:B:779:LYS:HG2	1:B:820:LYS:HB2	1.85	0.57
1:A:725:LEU:HB3	1:A:738:VAL:HG11	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:ARG:HH11	1:B:155:GLN:HB3	1.70	0.56
1:B:393:GLU:O	1:B:394:ASP:HB2	2.05	0.56
1:B:479:THR:O	1:B:594:THR:HG23	2.06	0.56
1:B:480:PRO:HG3	1:B:598:THR:HA	1.87	0.56
2:C:95:GLY:HA3	2:C:108:ILE:HG21	1.87	0.56
1:A:137:ARG:HH11	1:A:155:GLN:HB3	1.71	0.56
2:D:54:GLN:OE1	2:D:105:PRO:HB3	2.05	0.56
1:B:566:THR:C	1:B:567:LEU:HD12	2.31	0.56
1:B:725:LEU:HB3	1:B:738:VAL:HG11	1.86	0.56
1:A:322:TYR:HB2	1:A:352:SER:HB2	1.87	0.56
1:A:531:ARG:HH11	1:A:725:LEU:HD21	1.71	0.56
1:A:393:GLU:O	1:A:394:ASP:HB2	2.06	0.55
1:A:421:LEU:H	1:A:421:LEU:HD13	1.71	0.55
1:B:480:PRO:HD3	1:B:594:THR:HA	1.89	0.55
1:B:114:ASP:OD2	1:B:639:ARG:NH2	2.39	0.54
1:B:475:MET:HA	1:B:478:VAL:HG23	1.89	0.54
1:B:531:ARG:HH11	1:B:725:LEU:HD21	1.72	0.54
1:B:548:THR:CG2	1:B:549:THR:N	2.67	0.54
1:B:765:ASP:O	1:B:790:PRO:HD2	2.06	0.54
2:C:165:THR:OG1	2:C:168:GLN:HG3	2.07	0.54
1:A:126:ILE:HG23	1:A:206:VAL:HB	1.89	0.54
1:A:212:THR:HG22	1:A:222:LEU:O	2.07	0.54
2:C:84:THR:HG21	2:C:127:GLY:HA2	1.89	0.54
1:B:199:ASP:OD2	1:B:280:ARG:NH1	2.40	0.54
1:B:266:LEU:N	1:B:266:LEU:HD23	2.22	0.54
1:B:283:GLY:HA2	1:B:321:HIS:CB	2.37	0.54
1:A:114:ASP:OD2	1:A:639:ARG:NH2	2.40	0.54
1:A:477:GLY:HA2	1:A:480:PRO:HB3	1.90	0.54
1:B:319:ASP:HB3	1:B:353:PRO:HB2	1.88	0.54
1:B:186:LYS:HD2	1:B:411:ASP:OD1	2.08	0.54
1:B:212:THR:HG22	1:B:222:LEU:O	2.08	0.54
1:B:421:LEU:HD13	1:B:421:LEU:H	1.71	0.54
1:A:319:ASP:HB3	1:A:353:PRO:HB2	1.90	0.53
1:B:456:ASN:HB3	1:B:492:ASN:OD1	2.08	0.53
1:A:199:ASP:OD2	1:A:280:ARG:NH1	2.41	0.53
2:D:84:THR:HG21	2:D:127:GLY:HA2	1.90	0.53
1:A:181:ARG:HH12	1:A:219:ALA:H	1.56	0.53
1:A:480:PRO:HD3	1:A:594:THR:HA	1.88	0.53
2:D:76:THR:HG22	4:D:189:HOH:O	2.09	0.53
1:A:322:TYR:CB	1:A:352:SER:HB2	2.39	0.53
2:C:46:TYR:HB3	2:C:54:GLN:HG2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:MET:HE3	1:A:405:TYR:HB2	1.91	0.53
1:B:347:GLN:NE2	1:B:380:MET:HE1	2.24	0.53
2:D:15:SER:HA	2:D:165:THR:HA	1.91	0.53
1:A:516:GLY:HA3	1:A:597:LEU:HD11	1.90	0.53
1:B:779:LYS:HG2	1:B:820:LYS:HZ3	1.73	0.53
1:A:403:LYS:O	1:A:404:LEU:HD12	2.09	0.52
1:B:516:GLY:HA3	1:B:597:LEU:HD11	1.90	0.52
1:B:322:TYR:HB2	1:B:352:SER:HB2	1.89	0.52
1:B:139:ALA:O	1:B:142:ILE:HG12	2.09	0.52
1:B:120:PRO:O	1:B:121:ARG:HB3	2.09	0.52
1:B:497:TYR:HB3	1:B:501:LEU:HB3	1.91	0.52
1:B:375:GLY:HA2	1:B:416:TYR:CD1	2.45	0.52
1:B:725:LEU:HB3	1:B:738:VAL:CG1	2.40	0.52
1:B:790:PRO:O	1:B:809:LYS:HB3	2.08	0.52
2:D:118:LEU:O	2:D:119:ASN:C	2.53	0.51
2:C:59:SER:O	2:C:63:GLN:HA	2.10	0.51
1:A:790:PRO:O	1:A:809:LYS:HB3	2.11	0.51
1:B:189:HIS:HB2	1:B:191:GLN:NE2	2.26	0.51
1:B:180:MET:HE3	1:B:405:TYR:HB2	1.92	0.51
2:C:15:SER:HA	2:C:165:THR:HA	1.91	0.51
1:B:303:GLY:O	1:B:304:ASN:HB2	2.11	0.51
1:B:181:ARG:HH12	1:B:219:ALA:H	1.59	0.51
1:B:175:MET:HE2	1:B:196:MET:HG2	1.93	0.51
1:B:531:ARG:HH11	1:B:725:LEU:HD11	1.76	0.51
2:D:59:SER:O	2:D:63:GLN:HA	2.10	0.51
1:A:303:GLY:O	1:A:304:ASN:HB2	2.11	0.51
1:A:444:ARG:HG3	1:A:454:ARG:HG3	1.92	0.50
1:A:186:LYS:HD2	1:A:411:ASP:OD1	2.11	0.50
2:D:120:LEU:HD13	2:D:120:LEU:C	2.36	0.50
1:B:126:ILE:HG23	1:B:206:VAL:HB	1.93	0.50
1:B:327:ARG:HB2	3:B:866:GOL:H2	1.93	0.50
1:B:593:ILE:HD12	1:B:593:ILE:N	2.24	0.50
1:A:300:ASN:HB3	1:A:302:THR:HG23	1.94	0.50
1:A:347:GLN:NE2	1:A:380:MET:HE1	2.26	0.50
1:A:589:ARG:HG3	1:A:589:ARG:O	2.11	0.50
1:B:661:ARG:NH2	1:B:716:SER:OG	2.44	0.50
1:A:725:LEU:HB3	1:A:738:VAL:CG1	2.41	0.50
2:C:1:PRO:HB3	2:C:119:ASN:HD21	1.76	0.50
1:B:798:PRO:HD2	1:B:801:TYR:CE1	2.47	0.50
2:C:54:GLN:OE1	2:C:105:PRO:HB3	2.11	0.50
2:C:118:LEU:O	2:C:119:ASN:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:122:SER:HB2	2:C:132:VAL:HG23	1.94	0.50
1:A:462:TYR:CE1	1:A:486:VAL:HG13	2.46	0.49
1:B:477:GLY:HA2	1:B:480:PRO:HB3	1.94	0.49
2:C:120:LEU:HD13	2:C:120:LEU:C	2.37	0.49
1:A:661:ARG:NH2	1:A:716:SER:OG	2.46	0.49
1:B:148:GLY:H	1:B:706:THR:HG21	1.76	0.49
1:A:479:THR:O	1:A:594:THR:HG23	2.12	0.49
2:C:1:PRO:CB	2:C:119:ASN:HD21	2.26	0.49
1:A:139:ALA:O	1:A:142:ILE:HG12	2.13	0.49
2:D:95:GLY:HA3	2:D:108:ILE:HG21	1.95	0.49
1:A:410:GLN:NE2	1:A:429:ARG:HE	2.11	0.49
1:A:287:PRO:HG3	1:A:317:ILE:HD11	1.95	0.49
1:B:297:ARG:NH2	1:B:846:THR:O	2.46	0.49
1:B:444:ARG:HG3	1:B:454:ARG:HG3	1.94	0.49
2:D:80:GLU:HG2	2:D:81:PRO:HA	1.94	0.49
1:A:341:LEU:HD12	1:A:386:PHE:CE1	2.48	0.48
1:A:266:LEU:HD23	1:A:266:LEU:N	2.29	0.48
1:B:700:TYR:CZ	1:B:772:GLY:HA3	2.48	0.48
1:B:854:GLY:O	1:B:855:ARG:C	2.55	0.48
1:A:265:ALA:HB2	1:A:274:LEU:HD23	1.95	0.48
1:B:578:LEU:HD21	1:B:580:LEU:CD2	2.44	0.48
1:A:120:PRO:O	1:A:121:ARG:HB3	2.12	0.48
1:A:300:ASN:O	1:A:302:THR:HG23	2.13	0.48
2:C:62:ASN:O	2:C:63:GLN:HB2	2.13	0.48
1:B:191:GLN:HG2	1:B:845:GLU:CD	2.38	0.48
1:A:297:ARG:NH2	1:A:846:THR:O	2.47	0.48
1:B:184:PHE:HA	1:B:432:LEU:HD23	1.94	0.48
1:B:322:TYR:CB	1:B:352:SER:HB2	2.44	0.48
1:B:669:PRO:HB3	2:D:44:GLY:HA3	1.95	0.48
2:C:43:GLY:HA3	2:C:55:TYR:OH	2.14	0.48
1:B:525:LEU:HD12	1:B:532:TYR:HB2	1.95	0.47
1:A:175:MET:HE2	1:A:196:MET:HG2	1.95	0.47
2:D:43:GLY:HA3	2:D:55:TYR:OH	2.13	0.47
1:B:525:LEU:HD11	1:B:546:CYS:HB3	1.96	0.47
1:A:507:LEU:HD13	3:A:866:GOL:H32	1.96	0.47
1:B:341:LEU:HD12	1:B:386:PHE:CE1	2.48	0.47
1:B:589:ARG:HA	1:B:590:PRO:HD3	1.79	0.47
1:A:375:GLY:HA2	1:A:416:TYR:CD1	2.50	0.47
1:A:405:TYR:CZ	1:A:436:GLY:HA3	2.50	0.47
1:B:199:ASP:O	1:B:199:ASP:OD2	2.31	0.47
1:B:405:TYR:CZ	1:B:436:GLY:HA3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:THR:C	1:A:567:LEU:HD12	2.39	0.47
1:A:578:LEU:HD21	1:A:580:LEU:HD21	1.96	0.47
1:B:538:CYS:HB3	1:B:736:PHE:HB2	1.97	0.47
1:A:358:LEU:HD13	1:A:371:TRP:CZ2	2.50	0.47
1:A:564:SER:HB3	1:A:586:LYS:O	2.15	0.47
1:B:273:ILE:HD13	1:B:331:VAL:HG22	1.97	0.47
1:B:300:ASN:HB3	1:B:302:THR:HG23	1.95	0.47
1:A:189:HIS:HB2	1:A:191:GLN:NE2	2.29	0.47
1:A:189:HIS:HB2	1:A:191:GLN:CD	2.40	0.47
1:A:475:MET:SD	1:A:478:VAL:HG21	2.55	0.47
1:A:720:TRP:O	1:A:721:LEU:HB2	2.15	0.47
1:A:496:ASP:OD1	1:A:502:THR:HG23	2.14	0.47
1:B:172:ARG:HH12	1:B:655:ILE:HD13	1.76	0.47
1:B:496:ASP:OD1	1:B:502:THR:HG23	2.15	0.47
1:A:456:ASN:HB3	1:A:492:ASN:OD1	2.15	0.47
1:A:578:LEU:HD21	1:A:580:LEU:CD2	2.45	0.47
1:A:531:ARG:HH11	1:A:725:LEU:HD11	1.80	0.46
1:B:189:HIS:HB2	1:B:191:GLN:CD	2.40	0.46
1:A:661:ARG:HA	1:A:661:ARG:HD3	1.83	0.46
1:B:662:ASN:ND2	1:B:718:LYS:HE3	2.30	0.46
1:B:589:ARG:O	1:B:589:ARG:HG3	2.14	0.46
1:A:191:GLN:HG2	1:A:845:GLU:CD	2.41	0.46
1:A:780:LEU:HD23	1:A:819:TYR:HD1	1.81	0.46
1:B:336:PRO:O	1:B:339:GLN:HG3	2.16	0.46
1:A:336:PRO:O	1:A:339:GLN:HG3	2.15	0.46
1:A:421:LEU:HD23	1:A:422:LEU:HD23	1.97	0.46
1:B:768:SER:HA	1:B:786:VAL:O	2.15	0.46
2:D:120:LEU:HD11	2:D:131:VAL:CG1	2.45	0.46
1:A:538:CYS:HB3	1:A:736:PHE:HB2	1.98	0.46
1:A:620:ARG:HD2	1:A:620:ARG:O	2.16	0.46
1:A:827:LEU:HD23	1:A:827:LEU:N	2.30	0.46
2:C:80:GLU:HG2	2:C:81:PRO:HA	1.96	0.46
1:B:421:LEU:HD23	1:B:422:LEU:HD23	1.97	0.46
1:A:507:LEU:HD12	1:A:507:LEU:O	2.15	0.46
1:A:662:ASN:ND2	1:A:718:LYS:HE3	2.31	0.46
1:A:117:TYR:CG	1:A:641:VAL:HG22	2.51	0.46
1:A:700:TYR:CZ	1:A:772:GLY:HA3	2.50	0.46
1:B:176:ASN:OD1	1:B:227:THR:HA	2.15	0.46
1:B:462:TYR:CE1	1:B:486:VAL:HG13	2.51	0.46
1:B:593:ILE:H	1:B:593:ILE:CD1	2.25	0.46
1:A:274:LEU:C	1:A:274:LEU:HD13	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:LEU:HB3	1:A:336:PRO:CD	2.46	0.45
1:B:475:MET:SD	1:B:602:ALA:HA	2.56	0.45
1:B:508:ARG:O	1:B:563:LEU:HD12	2.16	0.45
1:A:539:LYS:HA	1:A:734:GLY:CA	2.46	0.45
1:A:589:ARG:HA	1:A:590:PRO:HD3	1.82	0.45
1:B:520:LEU:C	1:B:520:LEU:HD23	2.40	0.45
1:A:500:TRP:O	1:A:571:VAL:HA	2.16	0.45
1:A:507:LEU:HD13	3:A:866:GOL:C3	2.47	0.45
1:B:308:TYR:CD1	1:B:369:LEU:HD13	2.51	0.45
1:B:578:LEU:HD21	1:B:580:LEU:HD21	1.97	0.45
1:A:115:TRP:CD1	1:A:115:TRP:H	2.34	0.45
1:A:778:ARG:O	1:A:778:ARG:HG3	2.17	0.45
1:A:657:LEU:O	1:A:755:GLN:O	2.33	0.45
1:A:243:LEU:HD23	1:A:243:LEU:C	2.42	0.45
1:B:184:PHE:O	1:B:194:GLY:HA2	2.17	0.45
1:B:358:LEU:HD13	1:B:371:TRP:CZ2	2.52	0.45
1:B:589:ARG:NH1	1:B:655:ILE:HD12	2.30	0.45
1:B:728:GLY:HA3	1:B:737:TYR:CE2	2.52	0.45
2:D:110:VAL:HG22	2:D:110:VAL:O	2.16	0.45
1:A:231:VAL:HG11	1:A:263:ILE:HD13	1.98	0.45
1:B:500:TRP:O	1:B:571:VAL:HA	2.17	0.45
1:A:462:TYR:CZ	1:A:486:VAL:CG1	3.00	0.45
1:A:295:ASN:O	1:A:299:ASN:HB3	2.17	0.44
1:B:360:ASN:HB3	2:D:80:GLU:HG3	1.98	0.44
1:B:479:THR:HB	1:B:480:PRO:O	2.17	0.44
1:B:720:TRP:O	1:B:721:LEU:HB2	2.17	0.44
1:A:656:ASN:O	1:A:676:TYR:HA	2.17	0.44
1:A:853:ARG:NH1	1:A:856:THR:HG21	2.25	0.44
1:B:296:ILE:HG22	1:B:804:LEU:HD13	1.99	0.44
1:A:617:GLU:OE1	1:A:654:TYR:HA	2.17	0.44
1:B:175:MET:HE2	1:B:196:MET:SD	2.58	0.44
1:A:589:ARG:NH1	1:A:655:ILE:HD12	2.32	0.44
1:A:831:VAL:HG22	1:A:857:VAL:HG22	1.99	0.44
1:A:497:TYR:HB3	1:A:501:LEU:HB3	1.98	0.44
1:A:854:GLY:O	1:A:855:ARG:C	2.61	0.44
1:B:504:GLU:HB3	1:B:568:ALA:HB3	1.98	0.44
1:B:780:LEU:HD23	1:B:819:TYR:HD1	1.82	0.44
1:A:148:GLY:H	1:A:706:THR:HG21	1.81	0.44
1:A:564:SER:HA	1:A:565:PRO:HD3	1.75	0.44
1:B:732:ARG:HA	1:B:736:PHE:CZ	2.53	0.44
1:A:199:ASP:O	1:A:199:ASP:OD2	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:577:TRP:CZ3	1:A:630:GLN:HG2	2.52	0.44
1:B:265:ALA:HB2	1:B:274:LEU:HD23	2.00	0.44
1:B:274:LEU:HD13	1:B:274:LEU:C	2.43	0.44
1:A:143:LEU:HD12	1:A:143:LEU:HA	1.83	0.44
1:B:531:ARG:NH1	1:B:725:LEU:HD11	2.33	0.44
1:A:516:GLY:HA3	1:A:597:LEU:CD1	2.47	0.44
1:A:599:ASN:CG	1:A:599:ASN:O	2.60	0.44
1:B:266:LEU:O	1:B:266:LEU:HG	2.17	0.44
1:B:403:LYS:O	1:B:404:LEU:HD12	2.18	0.44
2:C:22:GLN:O	2:C:26:THR:HG23	2.17	0.44
1:A:508:ARG:O	1:A:563:LEU:HD12	2.18	0.43
1:B:498:ASP:HB2	1:B:500:TRP:CD1	2.53	0.43
1:B:542:ARG:N	1:B:542:ARG:HD2	2.33	0.43
1:A:299:ASN:O	1:A:300:ASN:HB2	2.18	0.43
1:B:287:PRO:HG3	1:B:317:ILE:HD11	2.00	0.43
1:B:614:LEU:HD23	1:B:614:LEU:HA	1.83	0.43
1:B:832:GLU:HB2	1:B:856:THR:HB	1.98	0.43
1:B:177:ILE:HD12	1:B:346:LEU:HD23	2.00	0.43
1:B:243:LEU:C	1:B:243:LEU:HD23	2.43	0.43
2:C:123:LEU:H	2:C:123:LEU:CD2	2.29	0.43
1:A:489:LEU:HA	1:A:489:LEU:HD12	1.80	0.43
1:A:717:ASN:O	1:A:747:PHE:O	2.36	0.43
1:B:802:PRO:HG3	2:D:77:LEU:HD23	2.01	0.43
1:A:138:HIS:O	1:A:139:ALA:C	2.62	0.43
1:A:807:TRP:CZ2	1:A:843:TYR:HA	2.53	0.43
1:B:516:GLY:HA3	1:B:597:LEU:CD1	2.48	0.43
1:A:640:LEU:HD23	1:A:694:TYR:HB2	2.00	0.43
1:A:116:VAL:HG21	1:A:125:VAL:HG12	2.01	0.43
1:A:176:ASN:OD1	1:A:227:THR:HA	2.19	0.43
1:A:525:LEU:HD12	1:A:532:TYR:HB2	2.00	0.43
1:B:137:ARG:HB2	1:B:282:LEU:HD13	2.01	0.43
1:B:411:ASP:OD2	1:B:411:ASP:C	2.61	0.43
1:A:119:GLU:HA	1:A:120:PRO:HD3	1.78	0.43
1:A:308:TYR:CD1	1:A:369:LEU:HD13	2.54	0.43
1:A:717:ASN:C	1:A:719:ALA:H	2.26	0.43
1:A:768:SER:HA	1:A:786:VAL:O	2.19	0.43
1:B:115:TRP:CD1	1:B:115:TRP:H	2.36	0.43
1:B:117:TYR:CG	1:B:641:VAL:HG22	2.54	0.43
1:B:231:VAL:HG11	1:B:263:ILE:HD13	2.00	0.43
1:B:295:ASN:O	1:B:299:ASN:HB3	2.19	0.43
1:B:534:ILE:HG23	1:B:535:ASP:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:41:ASN:HD22	2:C:60:THR:HB	1.82	0.43
2:D:46:TYR:HB3	2:D:54:GLN:CG	2.47	0.43
1:A:595:GLU:HA	1:A:676:TYR:CD1	2.54	0.43
1:B:419:SER:OG	1:B:422:LEU:HB2	2.19	0.43
1:B:717:ASN:O	1:B:747:PHE:O	2.37	0.43
2:C:120:LEU:HD11	2:C:131:VAL:CG1	2.48	0.43
1:B:462:TYR:CZ	1:B:486:VAL:CG1	3.02	0.42
1:A:492:ASN:HB3	1:A:506:GLY:HA3	2.01	0.42
1:B:119:GLU:HA	1:B:120:PRO:HD3	1.77	0.42
1:B:525:LEU:CD1	1:B:546:CYS:HB3	2.49	0.42
1:B:640:LEU:HD23	1:B:694:TYR:HB2	2.00	0.42
2:D:39:ASP:HA	2:D:40:ALA:HA	1.47	0.42
2:D:73:LEU:HB3	2:D:85:LEU:HD11	2.00	0.42
2:D:131:VAL:O	2:D:135:VAL:HG12	2.19	0.42
1:A:502:THR:C	1:A:503:LEU:HD12	2.44	0.42
1:B:522:TYR:HB2	1:B:664:PRO:O	2.19	0.42
1:A:302:THR:HG21	2:C:124:GLN:OE1	2.20	0.42
2:D:123:LEU:H	2:D:123:LEU:CD2	2.30	0.42
1:A:411:ASP:OD2	1:A:411:ASP:C	2.62	0.42
1:A:780:LEU:HD22	1:A:780:LEU:HA	1.82	0.42
1:B:157:ASP:HA	1:B:158:PRO:HD3	1.79	0.42
1:B:341:LEU:HD12	1:B:386:PHE:CZ	2.54	0.42
1:A:176:ASN:HD22	1:A:179:GLY:HA2	1.84	0.42
1:A:335:LEU:HB2	1:A:339:GLN:HB2	2.01	0.42
1:A:525:LEU:HD11	1:A:546:CYS:HB3	2.01	0.42
1:B:154:SER:C	1:B:156:GLN:H	2.27	0.42
1:B:489:LEU:HD12	1:B:489:LEU:HA	1.88	0.42
1:B:717:ASN:C	1:B:719:ALA:H	2.27	0.42
1:A:762:LEU:N	1:A:762:LEU:HD12	2.35	0.42
1:B:308:TYR:HB3	1:B:369:LEU:HD22	2.01	0.42
1:B:335:LEU:HB3	1:B:336:PRO:CD	2.50	0.42
1:B:580:LEU:HD23	1:B:626:PHE:HB3	2.01	0.42
1:B:656:ASN:O	1:B:676:TYR:HA	2.19	0.42
2:D:166:PHE:HA	2:D:169:VAL:HG22	2.02	0.42
1:A:475:MET:SD	1:A:602:ALA:HA	2.60	0.42
1:B:138:HIS:O	1:B:139:ALA:C	2.60	0.42
1:A:614:LEU:HD23	1:A:614:LEU:HA	1.82	0.42
1:B:522:TYR:HA	1:B:523:PRO:HD3	1.86	0.42
1:A:172:ARG:HH12	1:A:655:ILE:HD13	1.82	0.41
1:A:360:ASN:ND2	2:C:81:PRO:HA	2.35	0.41
1:A:419:SER:OG	1:A:422:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:SER:HB2	1:A:478:VAL:HG12	2.02	0.41
1:B:639:ARG:NH1	1:B:693:ASN:OD1	2.52	0.41
2:D:120:LEU:HD11	2:D:131:VAL:HG12	2.03	0.41
1:A:160:LEU:O	1:A:175:MET:HE1	2.20	0.41
1:A:302:THR:HB	2:C:125:ALA:HB2	2.02	0.41
1:A:728:GLY:HA3	1:A:737:TYR:CE2	2.55	0.41
1:B:328:LEU:HD12	1:B:329:ALA:H	1.85	0.41
1:B:762:LEU:N	1:B:762:LEU:HD12	2.35	0.41
2:C:46:TYR:HB3	2:C:54:GLN:CG	2.49	0.41
2:D:19:TYR:HD2	2:D:20:LEU:HD12	1.85	0.41
1:A:405:TYR:CE2	1:A:436:GLY:HA3	2.56	0.41
1:A:475:MET:C	1:A:477:GLY:H	2.29	0.41
1:A:655:ILE:HG22	1:A:678:ASN:ND2	2.35	0.41
1:B:300:ASN:C	1:B:302:THR:H	2.28	0.41
1:B:659:ILE:HG22	1:B:674:ALA:HB2	2.02	0.41
1:B:793:GLN:HA	1:B:805:ALA:O	2.20	0.41
1:B:802:PRO:O	1:B:847:LEU:HD13	2.20	0.41
1:A:273:ILE:HD13	1:A:331:VAL:HG22	2.01	0.41
1:A:572:ARG:HA	1:A:573:PRO:HD3	1.89	0.41
1:B:335:LEU:HB2	1:B:339:GLN:HB2	2.01	0.41
1:B:541:LEU:HD23	1:B:542:ARG:HE	1.85	0.41
1:B:801:TYR:HA	1:B:802:PRO:HD3	1.77	0.41
1:B:807:TRP:CZ2	1:B:843:TYR:HA	2.55	0.41
2:C:110:VAL:O	2:C:110:VAL:HG22	2.20	0.41
1:A:167:ILE:CG2	1:A:172:ARG:HB3	2.51	0.41
1:A:479:THR:HB	1:A:480:PRO:O	2.19	0.41
1:A:531:ARG:NH1	1:A:725:LEU:HD11	2.36	0.41
1:B:216:MET:SD	1:B:438:GLN:HB2	2.60	0.41
1:B:364:ARG:HA	1:B:365:PRO:HD3	1.91	0.41
1:A:157:ASP:HA	1:A:158:PRO:HD3	1.80	0.41
1:A:534:ILE:HG23	1:A:535:ASP:N	2.36	0.41
1:B:300:ASN:O	1:B:302:THR:N	2.54	0.41
1:B:345:TYR:HA	1:B:383:ASN:O	2.19	0.41
1:A:137:ARG:HB2	1:A:282:LEU:HD13	2.02	0.41
1:A:282:LEU:HD12	1:A:322:TYR:CE1	2.56	0.41
1:A:525:LEU:CD1	1:A:546:CYS:HB3	2.51	0.41
1:A:558:ARG:NH2	1:A:614:LEU:O	2.53	0.41
1:A:341:LEU:HD12	1:A:386:PHE:CZ	2.56	0.41
1:A:504:GLU:HB3	1:A:568:ALA:HB3	2.02	0.41
1:A:542:ARG:N	1:A:542:ARG:HD2	2.36	0.41
1:A:580:LEU:HD23	1:A:626:PHE:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:732:ARG:HA	1:A:736:PHE:CZ	2.56	0.41
1:B:282:LEU:HD12	1:B:322:TYR:CE1	2.56	0.41
1:B:364:ARG:O	1:B:364:ARG:CD	2.65	0.41
1:B:655:ILE:O	1:B:655:ILE:HG12	2.20	0.41
1:A:522:TYR:HB2	1:A:664:PRO:O	2.20	0.41
1:B:301:ASP:C	1:B:303:GLY:H	2.29	0.41
1:B:572:ARG:HA	1:B:573:PRO:HD3	1.89	0.41
1:B:657:LEU:O	1:B:755:GLN:O	2.38	0.41
1:A:184:PHE:O	1:A:194:GLY:HA2	2.21	0.40
1:A:770:THR:HA	1:A:784:VAL:O	2.22	0.40
1:B:347:GLN:HE21	1:B:380:MET:HE1	1.85	0.40
1:B:446:SER:C	1:B:447:LEU:HD12	2.46	0.40
1:B:127:SER:O	1:B:131:MET:HG3	2.21	0.40
1:B:288:GLY:HA3	1:B:837:ARG:C	2.46	0.40
1:A:731:SER:C	1:A:733:ARG:N	2.79	0.40
1:B:615:GLN:HG2	1:B:678:ASN:OD1	2.21	0.40
1:B:831:VAL:HG22	1:B:857:VAL:HG22	2.04	0.40
2:D:41:ASN:HD22	2:D:60:THR:HB	1.86	0.40
1:A:593:ILE:HD12	1:A:593:ILE:N	2.26	0.40
1:B:167:ILE:N	1:B:167:ILE:HD12	2.36	0.40
1:B:539:LYS:HA	1:B:734:GLY:CA	2.48	0.40
1:B:615:GLN:HA	1:B:616:PRO:HD3	1.96	0.40
1:A:475:MET:C	1:A:477:GLY:N	2.80	0.40
1:A:522:TYR:HA	1:A:523:PRO:HD3	1.87	0.40
1:B:380:MET:HE3	1:B:380:MET:HB3	1.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	751/865 (87%)	657 (88%)	84 (11%)	10 (1%)	9	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	751/865 (87%)	652 (87%)	89 (12%)	10 (1%)	9	38
2	C	159/206 (77%)	147 (92%)	9 (6%)	3 (2%)	6	30
2	D	159/206 (77%)	146 (92%)	10 (6%)	3 (2%)	6	30
All	All	1820/2142 (85%)	1602 (88%)	192 (10%)	26 (1%)	9	36

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	PRO
1	B	301	ASP
1	B	480	PRO
1	A	573	PRO
1	A	832	GLU
1	B	573	PRO
1	A	219	ALA
1	A	776	PHE
1	B	219	ALA
1	B	299	ASN
1	B	473	GLN
1	B	733	ARG
1	B	832	GLU
1	A	216	MET
1	A	299	ASN
1	A	473	GLN
1	A	654	TYR
1	B	776	PHE
2	C	119	ASN
2	D	124	GLN
2	D	5	VAL
1	A	303	GLY
2	C	57	ILE
1	B	303	GLY
2	C	64	VAL
2	D	64	VAL

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	616/695 (89%)	587 (95%)	29 (5%)	23	58
1	B	616/695 (89%)	585 (95%)	31 (5%)	22	56
2	C	124/158 (78%)	123 (99%)	1 (1%)	73	86
2	D	124/158 (78%)	123 (99%)	1 (1%)	73	86
All	All	1480/1706 (87%)	1418 (96%)	62 (4%)	26	61

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	VAL
1	A	121	ARG
1	A	125	VAL
1	A	126	ILE
1	A	177	ILE
1	A	273	ILE
1	A	318	PRO
1	A	340	ARG
1	A	409	THR
1	A	421	LEU
1	A	430	THR
1	A	442	THR
1	A	479	THR
1	A	486	VAL
1	A	507	LEU
1	A	511	ARG
1	A	525	LEU
1	A	564	SER
1	A	627	ASN
1	A	639	ARG
1	A	655	ILE
1	A	663	LYS
1	A	691	GLN
1	A	706	THR
1	A	712	ASN
1	A	720	TRP
1	A	729	ASP
1	A	758	SER
1	A	780	LEU
1	B	116	VAL

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Mol	Chain	Res	Type
1	B	121	ARG
1	B	125	VAL
1	B	126	ILE
1	B	177	ILE
1	B	273	ILE
1	B	318	PRO
1	B	340	ARG
1	B	409	THR
1	B	421	LEU
1	B	430	THR
1	B	442	THR
1	B	479	THR
1	B	486	VAL
1	B	507	LEU
1	B	511	ARG
1	B	525	LEU
1	B	564	SER
1	B	593	ILE
1	B	627	ASN
1	B	639	ARG
1	B	655	ILE
1	B	663	LYS
1	B	691	GLN
1	B	706	THR
1	B	712	ASN
1	B	720	TRP
1	B	729	ASP
1	B	758	SER
1	B	780	LEU
1	B	832	GLU
2	C	110	VAL
2	D	110	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	HIS
1	A	248	HIS
1	A	257	HIS
1	A	347	GLN
1	A	438	GLN
1	A	629	GLN

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Mol	Chain	Res	Type
1	A	833	ASN
1	B	248	HIS
1	B	257	HIS
1	B	347	GLN
1	B	599	ASN
1	B	629	GLN
1	B	833	ASN
2	C	41	ASN
2	C	119	ASN
2	D	41	ASN

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 ⓘ

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	B	868	-	5,5,5	0.42	0	5,5,5	0.84	0
3	GOL	B	866	-	5,5,5	0.54	0	5,5,5	0.42	0
3	GOL	B	869	-	5,5,5	0.43	0	5,5,5	0.45	0
3	GOL	A	866	-	5,5,5	0.44	0	5,5,5	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	B	867	-	5,5,5	0.48	0	5,5,5	0.47	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	868	-	-	2/4/4/4	-
3	GOL	B	866	-	-	2/4/4/4	-
3	GOL	B	869	-	-	0/4/4/4	-
3	GOL	A	866	-	-	2/4/4/4	-
3	GOL	B	867	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	866	GOL	O1-C1-C2-O2
3	A	866	GOL	O1-C1-C2-C3
3	B	866	GOL	O1-C1-C2-C3
3	B	867	GOL	O1-C1-C2-C3
3	B	868	GOL	O1-C1-C2-C3
3	B	866	GOL	O1-C1-C2-O2
3	B	867	GOL	O1-C1-C2-O2
3	B	868	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	866	GOL	1	0
3	A	866	GOL	2	0

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	753/865 (87%)	0.12	25 (3%)	49	28	44, 76, 123, 215	0
1	B	753/865 (87%)	0.10	25 (3%)	49	28	43, 75, 122, 206	0
2	C	163/206 (79%)	0.12	5 (3%)	51	30	36, 95, 119, 140	0
2	D	163/206 (79%)	0.11	4 (2%)	58	35	36, 94, 118, 140	0
All	All	1832/2142 (85%)	0.11	59 (3%)	50	29	36, 79, 122, 215	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	605	SER	5.8
2	D	1	PRO	5.2
2	C	28	GLY	4.9
1	A	603	HIS	4.9
1	B	603	HIS	4.6
1	B	292	ASP	4.5
1	A	605	SER	4.3
2	C	1	PRO	4.1
1	A	421	LEU	3.7
1	B	421	LEU	3.6
1	B	363	THR	3.6
1	B	474	GLY	3.5
1	B	577	TRP	3.4
1	A	299	ASN	3.2
1	A	652	ASP	3.1
1	A	779	LYS	2.9
1	B	479	THR	2.9
1	B	299	ASN	2.9
1	B	368	GLU	2.9
1	A	602	ALA	2.8
1	A	301	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	577	TRP	2.7
2	C	39	ASP	2.7
1	A	474	GLY	2.7
1	A	711	LYS	2.6
1	A	367	TYR	2.6
1	B	672	GLY	2.5
1	A	292	ASP	2.4
1	A	428	THR	2.4
1	A	479	THR	2.4
2	D	39	ASP	2.4
1	B	530	GLN	2.4
1	B	419	SER	2.4
1	B	291	GLY	2.4
1	B	832	GLU	2.4
1	A	368	GLU	2.3
1	A	832	GLU	2.3
1	B	779	LYS	2.3
2	C	131	VAL	2.3
2	D	119	ASN	2.3
1	B	361	LEU	2.2
1	A	212	THR	2.2
1	B	837	ARG	2.2
1	B	420	SER	2.1
1	A	291	GLY	2.1
1	A	575	VAL	2.1
1	A	361	LEU	2.1
2	D	173	THR	2.1
1	B	449	PRO	2.1
1	A	622	TRP	2.1
1	B	602	ALA	2.1
1	A	318	PRO	2.1
1	A	319	ASP	2.0
1	A	729	ASP	2.0
1	B	573	PRO	2.0
2	C	42	SER	2.0
1	B	634	TRP	2.0
1	B	699	PHE	2.0
1	B	734	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 [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
3	GOL	A	866	6/6	0.86	0.23	59,103,141,173	0
3	GOL	B	866	6/6	0.87	0.17	58,76,87,88	0
3	GOL	B	867	6/6	0.90	0.17	50,93,107,116	0
3	GOL	B	869	6/6	0.91	0.15	41,95,107,110	0
3	GOL	B	868	6/6	0.94	0.15	49,73,97,98	0

6.5 Other polymers [i](#)

There are no such residues in this entry.