



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 29, 2024 – 01:00 AM EDT

PDB ID : 3CSN  
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](mailto: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>.

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39



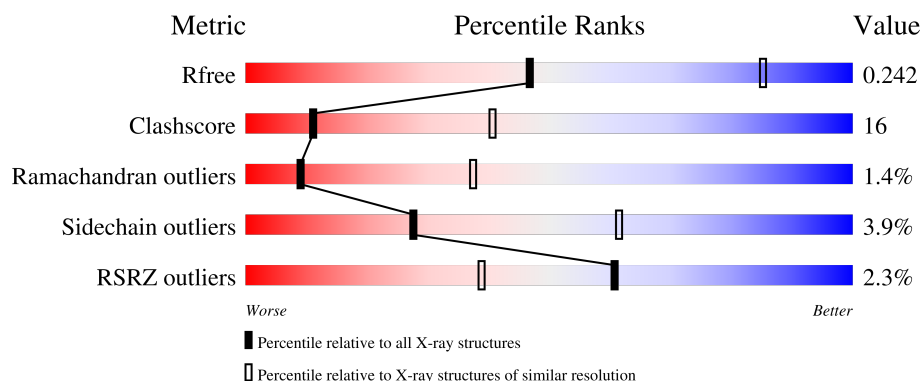
# 1 Overall quality at a glance

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))
$R_{free}$	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (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  $\geq 3$ , 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 (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).





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.

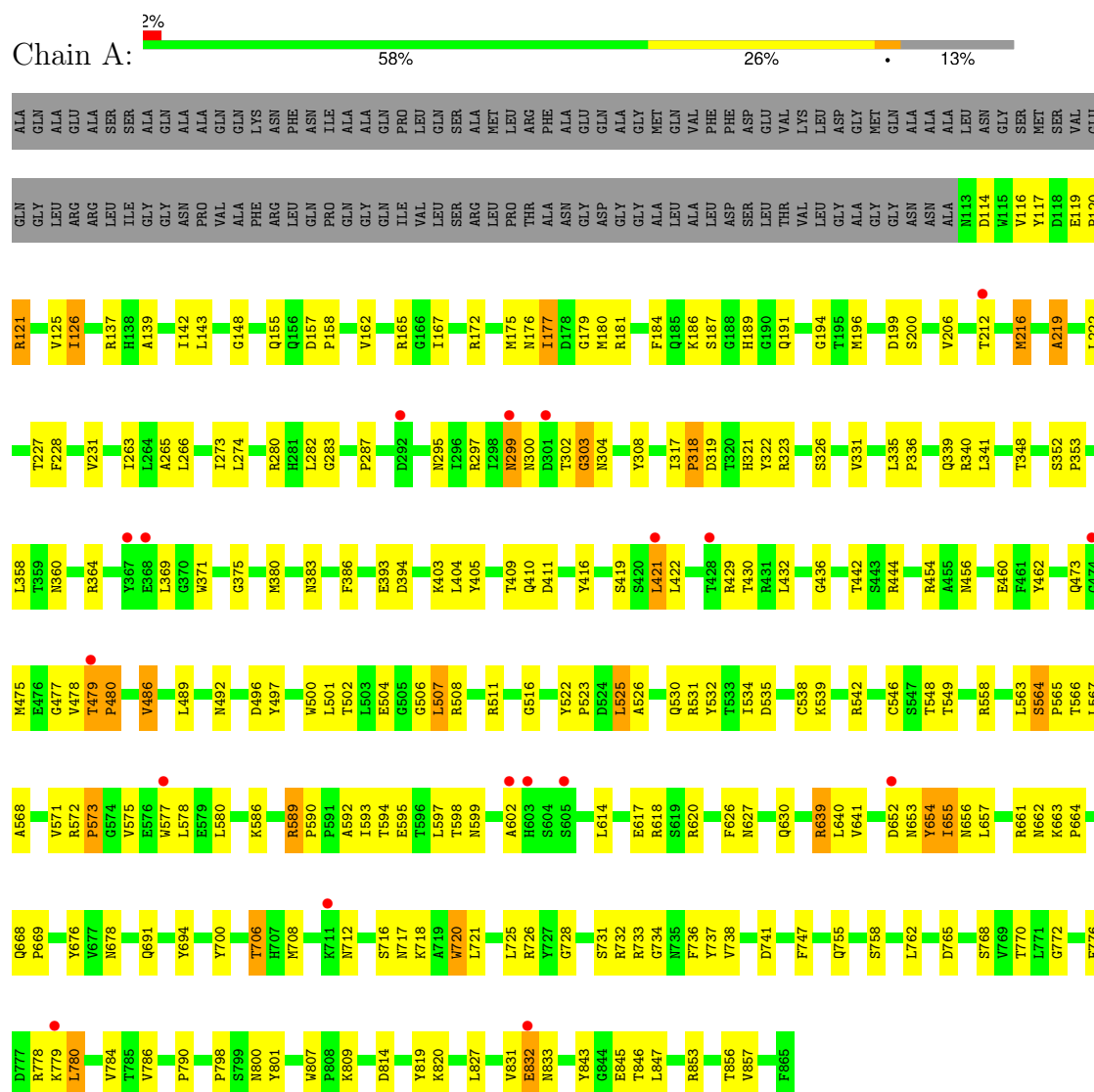
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total	O	0	0
			10	10		
4	B	7	Total	O	0	0
			7	7		
4	C	1	Total	O	0	0
			1	1		
4	D	1	Total	O	0	0
			1	1		



### 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.

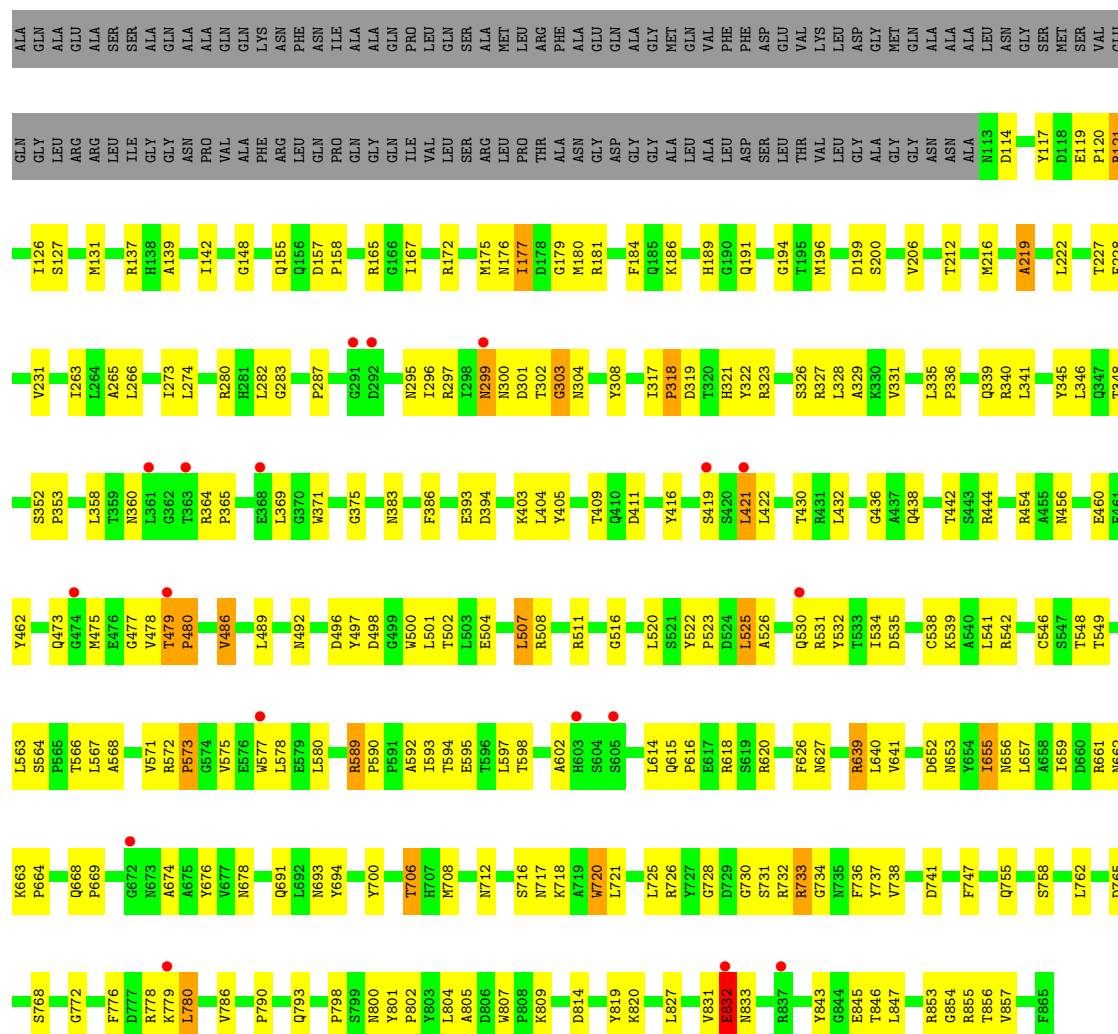
#### • Molecule 1: HasR protein



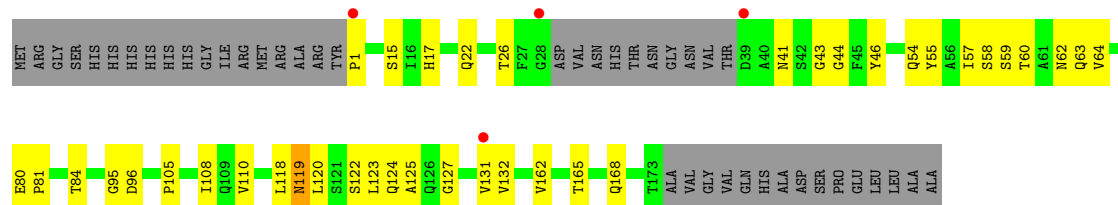
#### • Molecule 1: HasR protein



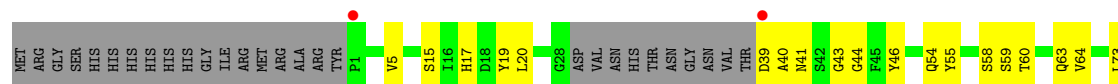




• Molecule 2: Hemophore HasA



• Molecule 2: Hemophore HasA









## 4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	3877 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.4	Xtriage
Anisotropy	0.543	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 66.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.49	0/6027	0.63	0/8188
1	B	0.50	0/6027	0.62	0/8188
2	C	0.42	0/1211	0.50	0/1649
2	D	0.43	0/1211	0.51	0/1649
All	All	0.48	0/14476	0.61	0/19674

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5889	0	5597	194	0
1	B	5889	0	5597	195	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	1	0
All	All	14195	0	13390	444	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 16.

All (444) 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:180:MET:HE1	1:A:383:ASN:HB3	1.49	0.95
1:A:779:LYS:HZ3	1:A:820:LYS:HG3	1.33	0.93
1:A:575:VAL:HG22	1:A:577:TRP:H	1.35	0.91
1:B:779:LYS:HZ3	1:B:820:LYS:HG3	1.37	0.89
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: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: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:548:THR:HG22	1:B:549:THR:N	1.98	0.78
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: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:B:175:MET:HE1	1:B:196:MET:HG2	1.67	0.73
1:A:216:MET:HE2	1:A:460:GLU:HB2	1.70	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:SER:OG	1:A:733:ARG:HG2	1.93	0.69
1:B:216:MET:HE2	1:B:460:GLU:HB2	1.75	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:620:ARG:C	1:A:620:ARG:HD2	2.13	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:B:300:ASN:O	1:B:302:THR:HG23	1.94	0.67
1:B:620:ARG:HD2	1:B:620:ARG:C	2.16	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
1:A:175:MET:HE1	1:A:196:MET:HG2	1.76	0.66
2:D:123:LEU:HD23	2:D:123:LEU:H	1.60	0.66
1:B:778:ARG:O	1:B:778:ARG:HG3	1.96	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: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: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
1:A:639:ARG:HD2	1:A:639:ARG:C	2.19	0.62
1:B:639:ARG:C	1:B:639:ARG:HD2	2.20	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:180:MET:CE	1:A:383:ASN:HB3	2.29	0.58
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:B:730:GLY:HA3	4:B:873:HOH:O	2.02	0.58
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:A:779:LYS:NZ	1:A:820:LYS:HG3	2.15	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:180:MET:HE3	1:B:405:TYR:HB2	1.86	0.56
2:D:54:GLN:OE1	2:D:105:PRO:HB3	2.05	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:A:403:LYS:C	1:A:404:LEU:HD12	2.28	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
1:B:180:MET:HE2	1:B:383:ASN:HB3	1.90	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:403:LYS:C	1:B:404:LEU:HD12	2.30	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: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
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:566:THR:C	1:B:567:LEU:HD12	2.31	0.51
1:A:589:ARG:HG3	1:A:589:ARG:O	2.11	0.51
1:A:779:LYS:HG2	1:A:820:LYS:HZ3	1.76	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
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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:C:62:ASN:O	2:C:63:GLN:HB2	2.13	0.48
1:A:120:PRO:O	1:A:121:ARG:HB3	2.12	0.48
1:B:779:LYS:HG2	1:B:820:LYS:HZ3	1.78	0.48
1:A:300:ASN:O	1:A:302:THR:HG23	2.13	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
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
1:A:578:LEU:HD21	1:A:580:LEU:HD21	1.96	0.47
1:A:720:TRP:O	1:A:721:LEU:HB2	2.15	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:475:MET:SD	1:A:478:VAL:HG21	2.55	0.47
2:D:118:LEU:O	2:D:119:ASN:C	2.53	0.47
1:A:496:ASP:OD1	1:A:502:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
2:D:120:LEU:HD13	2:D:120:LEU:C	2.36	0.46
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: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:B:720:TRP:O	1:B:721:LEU:HB2	2.17	0.45
2:C:118:LEU:O	2:C:119:ASN:C	2.54	0.45
1:A:778:ARG:O	1:A:778:ARG:HG3	2.17	0.45
1:A:165:ARG:HA	1:A:708:MET:CE	2.47	0.45
1:A:657:LEU:O	1:A:755:GLN:O	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:C:120:LEU:HD13	2:C:120:LEU:C	2.37	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: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:162:VAL:HG23	1:A:175:MET:HE3	2.00	0.44
1:A:199:ASP:O	1:A:199:ASP:OD2	2.35	0.44
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: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: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
1:B:854:GLY:O	1:B:855:ARG:C	2.55	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:165:ARG:HA	1:B:708:MET:CE	2.48	0.43
1:B:287:PRO:HG3	1:B:317:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:B:191:GLN:HG2	1:B:845:GLU:CD	2.38	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: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:768:SER:HA	1:A:786:VAL:O	2.19	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
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:566:THR:C	1:A:567:LEU:HD12	2.39	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:165:ARG:HA	1:B:708:MET:HE1	2.01	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:A:165:ARG:HA	1:A:708:MET:HE1	2.01	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:123:LEU:H	2:D:123:LEU:CD2	2.30	0.42
1:A:189:HIS:HB2	1:A:191:GLN:CD	2.40	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:489:LEU:HD12	1:B:489:LEU:HA	1.88	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:C:110:VAL:O	2:C:110:VAL:HG22	2.20	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:189:HIS:HB2	1:B:191:GLN:CD	2.40	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
1:A:187:SER:HB2	1:A:478:VAL:HG12	2.02	0.41
1:A:191:GLN:HG2	1:A:845:GLU:CD	2.41	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: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:655:ILE:HG22	1:A:678:ASN:ND2	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:380:MET:HB3	1:A:380:MET:HE2	1.88	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:274:LEU:HD13	1:A:274:LEU:C	2.41	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
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:520:LEU:C	1:B:520:LEU:HD23	2.40	0.41
1:B:655:ILE:O	1:B:655:ILE:HG12	2.20	0.41
1:B:779:LYS:NZ	1:B:820:LYS:HG3	2.20	0.41
1:A:522:TYR:HB2	1:A:664:PRO:O	2.20	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:599:ASN:CG	1:A:599:ASN:O	2.60	0.40
1:A:770:THR:HA	1:A:784:VAL:O	2.22	0.40
1:B:127:SER:O	1:B:131:MET:HG3	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:615:GLN:HA	1:B:616:PRO:HD3	1.96	0.40
1:A:522:TYR:HA	1:A:523:PRO:HD3	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	751/865 (87%)	657 (88%)	84 (11%)	10 (1%)	10	39
1	B	751/865 (87%)	652 (87%)	89 (12%)	10 (1%)	10	39
2	C	159/206 (77%)	147 (92%)	9 (6%)	3 (2%)	6	31
2	D	159/206 (77%)	146 (92%)	10 (6%)	3 (2%)	6	31
All	All	1820/2142 (85%)	1602 (88%)	192 (10%)	26 (1%)	9	37

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

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Mol	Chain	Res	Type
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%)	22	56
1	B	616/695 (89%)	587 (95%)	29 (5%)	22	56
2	C	124/158 (78%)	124 (100%)	0	100	100
2	D	124/158 (78%)	124 (100%)	0	100	100
All	All	1480/1706 (87%)	1422 (96%)	58 (4%)	27	61

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	ARG
1	A	126	ILE
1	A	177	ILE
1	A	318	PRO
1	A	323	ARG
1	A	340	ARG
1	A	409	THR
1	A	421	LEU

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Mol	Chain	Res	Type
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	589	ARG
1	A	618	ARG
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	758	SER
1	A	780	LEU
1	A	833	ASN
1	B	121	ARG
1	B	177	ILE
1	B	318	PRO
1	B	323	ARG
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	589	ARG
1	B	618	ARG
1	B	627	ASN
1	B	639	ARG
1	B	655	ILE
1	B	663	LYS

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Mol	Chain	Res	Type
1	B	691	GLN
1	B	706	THR
1	B	712	ASN
1	B	720	TRP
1	B	758	SER
1	B	780	LEU
1	B	832	GLU
1	B	833	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	410	GLN
1	A	629	GLN
1	A	833	ASN
1	B	833	ASN
2	C	119	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	869	-	5,5,5	0.43	0	5,5,5	0.45	0
3	GOL	B	867	-	5,5,5	0.48	0	5,5,5	0.47	0
3	GOL	B	866	-	5,5,5	0.54	0	5,5,5	0.42	0
3	GOL	A	866	-	5,5,5	0.44	0	5,5,5	0.64	0
3	GOL	B	868	-	5,5,5	0.42	0	5,5,5	0.84	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	869	-	-	0/4/4/4	-
3	GOL	B	867	-	-	2/4/4/4	-
3	GOL	B	866	-	-	2/4/4/4	-
3	GOL	A	866	-	-	2/4/4/4	-
3	GOL	B	868	-	-	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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	753/865 (87%)	-0.03	18 (2%) 59 37	44, 76, 123, 215	0
1	B	753/865 (87%)	-0.05	18 (2%) 59 37	43, 75, 122, 206	0
2	C	163/206 (79%)	-0.03	4 (2%) 58 36	36, 95, 119, 140	0
2	D	163/206 (79%)	-0.04	3 (1%) 67 45	36, 94, 118, 140	0
All	All	1832/2142 (85%)	-0.04	43 (2%) 61 39	36, 79, 122, 215	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	605	SER	5.6
2	D	1	PRO	5.0
2	C	28	GLY	4.7
1	A	603	HIS	4.7
1	B	603	HIS	4.4
1	B	292	ASP	4.3
1	A	605	SER	4.1
2	C	1	PRO	3.9
1	A	421	LEU	3.6
1	B	421	LEU	3.4
1	B	363	THR	3.4
1	B	474	GLY	3.4
1	B	577	TRP	3.1
1	A	299	ASN	3.1
1	A	652	ASP	3.0
1	A	779	LYS	2.8
1	B	368	GLU	2.8
1	B	479	THR	2.8
1	B	299	ASN	2.7
1	A	602	ALA	2.7
1	A	301	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	39	ASP	2.5
1	A	474	GLY	2.5
1	A	577	TRP	2.5
1	A	711	LYS	2.5
1	A	367	TYR	2.4
1	B	672	GLY	2.4
1	A	428	THR	2.3
1	A	479	THR	2.3
1	B	530	GLN	2.3
1	A	292	ASP	2.3
2	D	39	ASP	2.3
1	B	419	SER	2.3
1	B	832	GLU	2.2
1	B	291	GLY	2.2
1	A	368	GLU	2.2
1	B	779	LYS	2.2
1	A	832	GLU	2.2
2	C	131	VAL	2.2
2	D	119	ASN	2.1
1	B	361	LEU	2.1
1	B	837	ARG	2.1
1	A	212	THR	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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(Å <sup>2</sup> )	Q<0.9
3	GOL	A	866	6/6	0.86	0.23	59,103,141,173	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
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.