



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2024 – 08:36 AM EDT

PDB ID : 3EFO  
Title : Crystal Structure of the mammalian COPII-coat protein Sec23/24 bound to the transport signal sequence of syntaxin 5  
Authors : Goldberg, J.; Mancias, J.D.  
Deposited on : 2008-09-09  
Resolution : 2.70 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
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

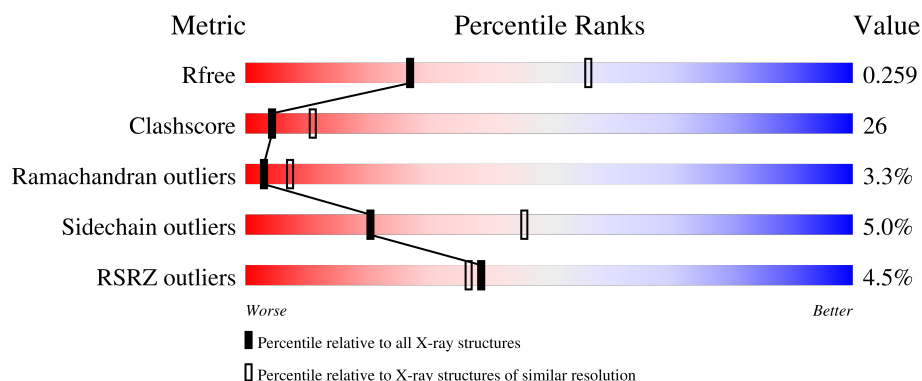
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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	765	
2	B	770	
3	C	7	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11927 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 Protein transport protein Sec23A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	716	Total	C	N	O	S	0	0	0
			5684	3623	975	1046	40			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	193	GLY	LYS	conflict	UNP Q15436

- Molecule 2 is a protein called SEC24 related gene family, member D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	767	Total	C	N	O	S	0	0	0
			6038	3841	1024	1119	54			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	ALA	-	expression tag	UNP Q8IYI7
B	2	MET	-	expression tag	UNP Q8IYI7
B	3	GLY	-	expression tag	UNP Q8IYI7

- Molecule 3 is a protein called Peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	7	Total	C	N	O	S	0	0	0
			53	32	7	12	2			

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Zn 1	0	0

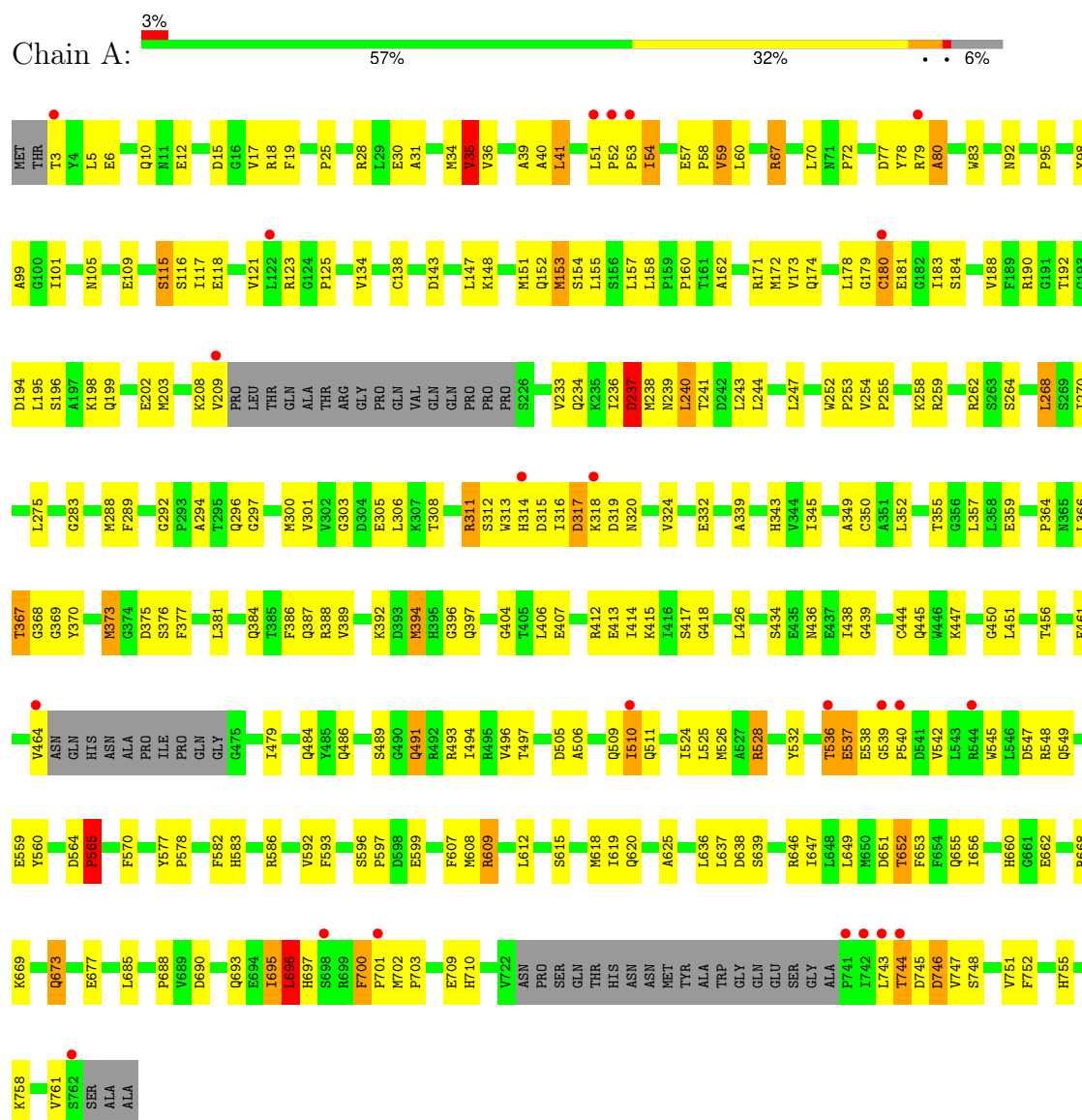
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	79	Total 79	O 79	0	0
5	B	71	Total 71	O 71	0	0

### 3 Residue-property plots

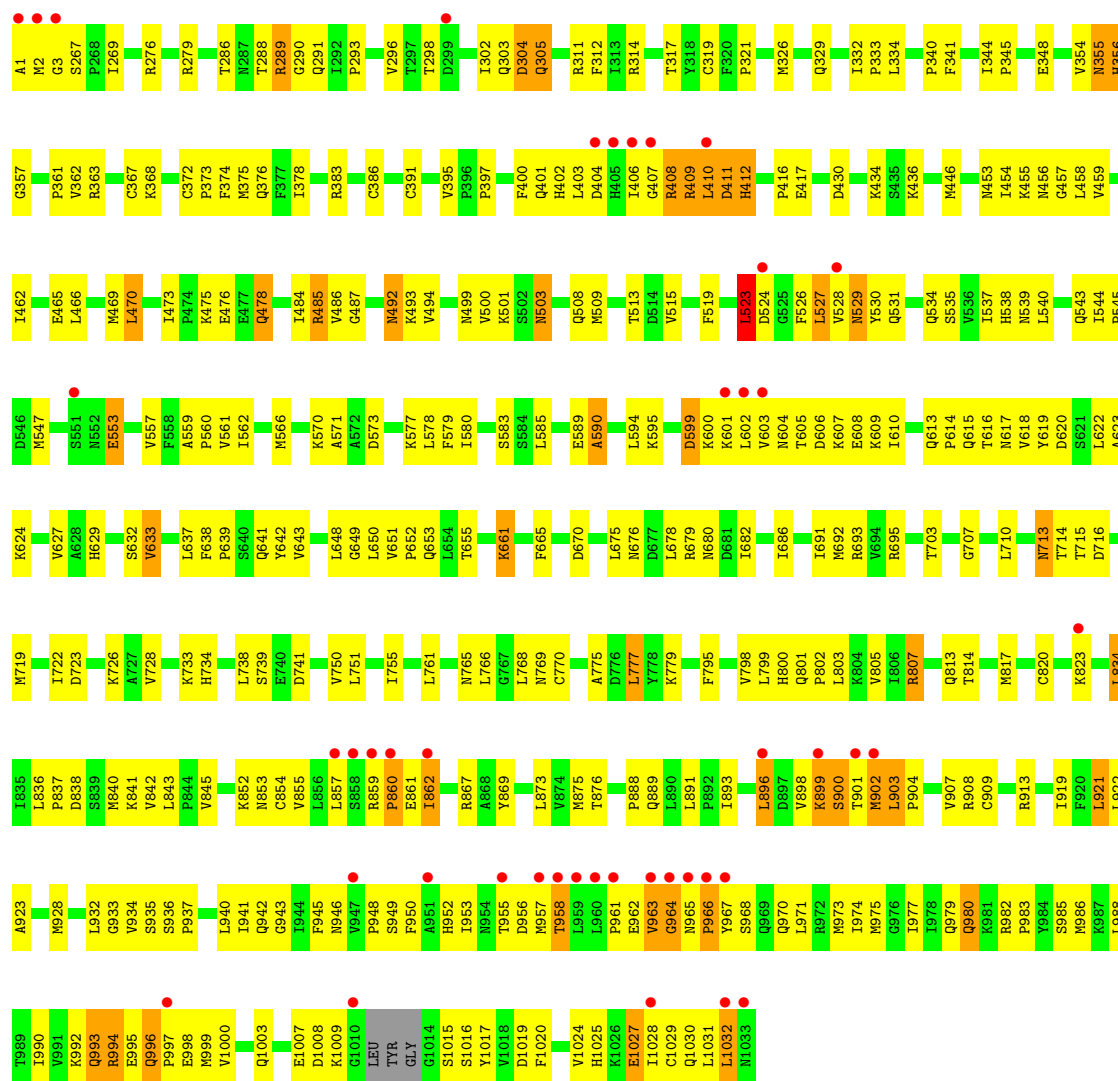
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Protein transport protein Sec23A



#### • Molecule 2: SEC24 related gene family, member D





### • Molecule 3: Peptide



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.06Å 140.83Å 152.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.70) 94.9 (50.00-2.70)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.13 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.211 , 0.261 0.210 , 0.259	Depositor DCC
$R_{free}$ test set	3050 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	51.1	Xtriage
Anisotropy	0.611	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 52.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11927	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.81% 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

### 5.1 Standard geometry

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

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	0.38	0/5817	0.66	3/7878 (0.0%)
2	B	0.38	0/6166	0.66	1/8351 (0.0%)
3	C	0.40	0/52	0.60	0/67
All	All	0.38	0/12035	0.66	4/16296 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	SER	N-CA-C	-7.63	90.40	111.00
1	A	652	THR	N-CA-C	-6.57	93.27	111.00
1	A	367	THR	N-CA-C	-5.82	95.28	111.00
2	B	523	LEU	N-CA-C	-5.21	96.93	111.00

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	5684	0	5636	246	0
2	B	6038	0	6038	376	0
3	C	53	0	50	5	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	0	0
5	A	79	0	0	10	0
5	B	71	0	0	7	0
All	All	11927	0	11724	617	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 26.

All (617) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:MET:HE1	2:B:836:LEU:HD12	1.30	1.14
1:A:747:VAL:HG12	1:A:748:SER:H	1.25	1.01
1:A:123:ARG:HG3	1:A:125:PRO:HD2	1.39	1.01
2:B:639:PRO:HB3	2:B:643:VAL:HG21	1.40	1.00
2:B:601:LYS:HB3	2:B:605:THR:HG21	1.44	0.99
2:B:996:GLN:HB3	2:B:997:PRO:HD2	1.45	0.98
1:A:54:ILE:HG13	1:A:117:ILE:HD11	1.41	0.97
2:B:2:MET:HE2	3:C:190:ILE:HD11	1.46	0.96
1:A:484:GLN:HG2	1:A:494:ILE:HG12	1.47	0.94
2:B:963:VAL:HG12	2:B:964:GLY:H	1.34	0.93
2:B:600:LYS:HD2	2:B:602:LEU:HD21	1.50	0.92
1:A:381:LEU:HA	1:A:702:MET:HE2	1.52	0.91
2:B:713:ASN:HD21	2:B:716:ASP:H	1.07	0.91
1:A:283:GLY:H	1:A:486:GLN:HE22	1.20	0.90
2:B:713:ASN:HD22	2:B:715:THR:H	1.17	0.89
1:A:51:LEU:HD12	1:A:52:PRO:HD2	1.54	0.88
2:B:901:THR:HG22	2:B:902:MET:H	1.38	0.86
2:B:713:ASN:ND2	2:B:715:THR:H	1.74	0.85
2:B:453:ASN:HD21	2:B:583:SER:HB3	1.40	0.85
1:A:296:GLN:HA	1:A:300:MET:HE2	1.59	0.84
2:B:2:MET:CE	2:B:836:LEU:HD12	2.06	0.84
2:B:453:ASN:ND2	2:B:583:SER:HB3	1.93	0.82
1:A:745:ASP:CG	1:A:746:ASP:H	1.82	0.82
2:B:713:ASN:ND2	2:B:716:ASP:H	1.79	0.79
1:A:18:ARG:NH1	1:A:612:LEU:HD22	1.98	0.79
2:B:974:ILE:HA	2:B:977:ILE:HG22	1.66	0.78
2:B:996:GLN:HB3	2:B:997:PRO:CD	2.13	0.78
1:A:609:ARG:HG3	1:A:609:ARG:HH11	1.48	0.78
1:A:297:GLY:H	1:A:300:MET:HB2	1.49	0.78
2:B:409:ARG:O	2:B:409:ARG:HG3	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:THR:HB	1:A:6:GLU:HG3	1.66	0.76
1:A:312:SER:O	1:A:316:ILE:HG22	1.85	0.76
1:A:297:GLY:N	1:A:300:MET:HB2	2.01	0.76
2:B:557:VAL:HA	5:B:1079:HOH:O	1.84	0.76
2:B:614:PRO:HG3	2:B:650:LEU:HD22	1.67	0.76
2:B:1030:GLN:C	2:B:1032:LEU:H	1.89	0.75
1:A:195:LEU:HD13	1:A:203:MET:HE1	1.66	0.75
1:A:656:ILE:HG13	1:A:695:ILE:HG21	1.68	0.75
1:A:528:ARG:HA	1:A:608:MET:HE1	1.66	0.75
1:A:239:ASN:HB3	5:A:845:HOH:O	1.86	0.75
2:B:500:VAL:HG11	2:B:537:ILE:HG12	1.68	0.75
1:A:375:ASP:HA	5:A:843:HOH:O	1.87	0.74
2:B:356:HIS:HD2	2:B:362:VAL:H	1.36	0.74
1:A:381:LEU:HA	1:A:702:MET:CE	2.18	0.74
1:A:3:THR:HG22	1:A:5:LEU:H	1.51	0.74
2:B:1000:VAL:HA	2:B:1003:GLN:HE21	1.51	0.73
1:A:198:LYS:HE2	1:A:202:GLU:OE2	1.88	0.73
2:B:933:GLY:O	2:B:936:SER:HB2	1.88	0.73
2:B:889:GLN:HG2	2:B:891:LEU:HD21	1.70	0.73
1:A:181:GLU:HG2	1:A:239:ASN:HD21	1.53	0.73
2:B:345:PRO:HB2	2:B:348:GLU:HG3	1.71	0.73
2:B:462:ILE:O	2:B:466:LEU:HB2	1.89	0.72
2:B:633:VAL:H	2:B:655:THR:HG21	1.54	0.72
2:B:637:LEU:HG	2:B:639:PRO:HD3	1.70	0.72
2:B:652:PRO:HA	2:B:655:THR:HG22	1.68	0.72
2:B:465:GLU:HG2	2:B:675:LEU:HD22	1.71	0.72
2:B:267:SER:HB3	2:B:908:ARG:HH21	1.55	0.72
1:A:596:SER:OG	1:A:599:GLU:HG3	1.88	0.72
2:B:595:LYS:H	2:B:615:GLN:HE22	1.36	0.72
2:B:901:THR:HB	2:B:970:GLN:HE21	1.53	0.72
2:B:692:MET:HE1	2:B:728:VAL:HG11	1.72	0.71
1:A:583:HIS:CD2	1:A:620:GLN:HE21	2.08	0.71
1:A:115:SER:O	1:A:116:SER:HB3	1.91	0.71
1:A:511:GLN:CD	1:A:511:GLN:H	1.92	0.70
2:B:600:LYS:HD2	2:B:602:LEU:CD2	2.19	0.70
2:B:454:ILE:HD13	2:B:459:VAL:HG21	1.73	0.70
1:A:583:HIS:HD2	1:A:620:GLN:HE21	1.39	0.70
2:B:963:VAL:HG12	2:B:964:GLY:N	2.07	0.70
1:A:369:GLY:O	1:A:609:ARG:NH2	2.24	0.70
2:B:997:PRO:O	2:B:999:MET:N	2.25	0.70
2:B:500:VAL:HG11	2:B:537:ILE:CG1	2.22	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:713:ASN:HD21	2:B:716:ASP:N	1.85	0.70
1:A:700:PHE:HB3	1:A:701:PRO:HD3	1.72	0.69
2:B:992:LYS:HD2	2:B:996:GLN:HE21	1.58	0.69
1:A:236:ILE:HG22	1:A:240:LEU:HB2	1.74	0.69
1:A:506:ALA:O	1:A:510:ILE:HG13	1.93	0.69
2:B:2:MET:CE	3:C:190:ILE:HD11	2.19	0.69
2:B:407:GLY:O	2:B:409:ARG:N	2.26	0.69
1:A:560:TYR:CD1	1:A:761:VAL:HG12	2.28	0.68
2:B:585:LEU:HD21	2:B:594:LEU:HB2	1.74	0.68
2:B:802:PRO:HB2	2:B:805:VAL:HG23	1.76	0.68
2:B:992:LYS:HD2	2:B:996:GLN:NE2	2.08	0.68
1:A:283:GLY:N	1:A:486:GLN:HE22	1.92	0.68
2:B:312:PHE:CZ	2:B:344:ILE:HD11	2.28	0.68
2:B:501:LYS:HD3	2:B:503:ASN:HD21	1.59	0.68
1:A:12:GLU:OE1	1:A:18:ARG:HD2	1.94	0.68
1:A:636:LEU:HG	1:A:638:ASP:HB2	1.76	0.68
1:A:652:THR:HG23	1:A:655:GLN:H	1.58	0.67
1:A:51:LEU:HD21	1:A:117:ILE:HA	1.74	0.67
1:A:656:ILE:HD11	1:A:695:ILE:HD13	1.74	0.67
1:A:116:SER:HA	1:A:496:VAL:O	1.93	0.67
2:B:602:LEU:HD11	2:B:859:ARG:HB2	1.75	0.67
1:A:404:GLY:HA2	1:A:484:GLN:O	1.94	0.67
2:B:842:VAL:HG12	2:B:842:VAL:O	1.94	0.67
2:B:901:THR:HG22	2:B:902:MET:N	2.09	0.67
2:B:493:LYS:HA	2:B:557:VAL:HG13	1.77	0.66
2:B:470:LEU:HD12	2:B:473:ILE:HD11	1.75	0.66
2:B:993:GLN:HG2	2:B:994:ARG:N	2.09	0.66
2:B:633:VAL:HG13	2:B:655:THR:HG21	1.78	0.66
1:A:747:VAL:HG12	1:A:748:SER:N	2.05	0.66
1:A:652:THR:CG2	1:A:655:GLN:H	2.10	0.65
1:A:745:ASP:CG	1:A:746:ASP:N	2.50	0.65
2:B:317:THR:HG22	2:B:319:CYS:H	1.61	0.65
1:A:700:PHE:O	1:A:702:MET:N	2.30	0.65
2:B:807:ARG:HG2	2:B:807:ARG:HH11	1.62	0.65
1:A:262:ARG:NH2	1:A:292:GLY:HA3	2.13	0.64
1:A:413:GLU:O	1:A:464:VAL:HG12	1.97	0.64
1:A:652:THR:HG21	1:A:655:GLN:HG2	1.79	0.64
2:B:267:SER:HB2	2:B:908:ARG:HE	1.61	0.64
2:B:485:ARG:HG3	5:B:1088:HOH:O	1.97	0.64
2:B:943:GLY:O	2:B:968:SER:HB2	1.97	0.64
2:B:948:PRO:HG2	2:B:952:HIS:ND1	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:627:VAL:HG21	2:B:710:LEU:HD23	1.79	0.64
2:B:600:LYS:O	2:B:600:LYS:HG3	1.98	0.64
2:B:605:THR:HG22	2:B:607:LYS:HB3	1.79	0.63
2:B:543:GLN:HB3	2:B:547:MET:CE	2.29	0.63
1:A:524:ILE:HD12	1:A:615:SER:HB3	1.80	0.63
1:A:30:GLU:OE1	1:A:506:ALA:HB3	1.98	0.63
2:B:719:MET:SD	2:B:722:ILE:HD12	2.38	0.63
2:B:919:ILE:HG23	2:B:932:LEU:HD23	1.81	0.63
2:B:958:THR:HG21	2:B:988:LEU:O	1.98	0.63
1:A:743:LEU:O	1:A:744:THR:HB	1.97	0.63
2:B:403:LEU:HA	2:B:409:ARG:HA	1.80	0.63
2:B:543:GLN:HG3	5:B:1102:HOH:O	1.97	0.63
2:B:600:LYS:HA	2:B:859:ARG:NH1	2.13	0.63
2:B:529:ASN:HD22	2:B:530:TYR:N	1.96	0.63
2:B:934:VAL:HG23	2:B:935:SER:N	2.14	0.62
1:A:559:GLU:O	1:A:560:TYR:HB3	1.99	0.62
2:B:616:THR:HG21	5:B:1047:HOH:O	1.99	0.62
1:A:297:GLY:CA	1:A:300:MET:HB2	2.30	0.62
2:B:500:VAL:HG12	2:B:500:VAL:O	2.00	0.62
2:B:355:ASN:ND2	2:B:357:GLY:H	1.96	0.62
2:B:456:ASN:OD1	2:B:458:LEU:HB2	1.99	0.62
2:B:974:ILE:HA	2:B:977:ILE:CG2	2.29	0.62
1:A:30:GLU:CD	1:A:506:ALA:HB3	2.20	0.62
2:B:355:ASN:HD22	2:B:356:HIS:N	1.98	0.62
2:B:602:LEU:HD23	2:B:602:LEU:N	2.15	0.62
2:B:942:GLN:HG2	2:B:948:PRO:HA	1.81	0.62
2:B:289:ARG:HD2	2:B:769:ASN:OD1	2.00	0.62
1:A:524:ILE:HD13	1:A:619:ILE:HD12	1.82	0.61
1:A:199:GLN:O	1:A:203:MET:HG3	2.00	0.61
1:A:195:LEU:CD1	1:A:203:MET:HE1	2.30	0.61
1:A:565:PRO:HG3	1:A:758:LYS:HA	1.83	0.61
2:B:501:LYS:CD	2:B:503:ASN:HD21	2.13	0.61
1:A:264:SER:HB2	1:A:294:ALA:HB2	1.81	0.61
1:A:583:HIS:CD2	1:A:620:GLN:HG3	2.35	0.61
2:B:378:ILE:HG12	2:B:383:ARG:O	2.01	0.61
2:B:639:PRO:CB	2:B:643:VAL:HG21	2.24	0.61
2:B:852:LYS:HE3	2:B:1015:SER:O	1.99	0.61
2:B:585:LEU:CD2	2:B:594:LEU:HB2	2.30	0.61
1:A:238:MET:O	1:A:241:THR:HG22	2.01	0.61
2:B:469:MET:HE3	2:B:679:ARG:HA	1.83	0.61
2:B:543:GLN:HB3	2:B:547:MET:HE3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:632:SER:HA	2:B:655:THR:OG1	2.00	0.61
1:A:190:ARG:HH12	2:B:519:PHE:HB3	1.65	0.60
2:B:963:VAL:O	2:B:964:GLY:O	2.19	0.60
2:B:616:THR:HG22	2:B:617:ASN:H	1.66	0.60
1:A:115:SER:O	1:A:116:SER:CB	2.50	0.60
2:B:269:ILE:HD11	2:B:907:VAL:C	2.22	0.60
2:B:979:GLN:HE22	2:B:986:MET:H	1.50	0.60
2:B:406:ILE:HG22	2:B:406:ILE:O	2.02	0.60
2:B:523:LEU:O	2:B:524:ASP:HB2	2.02	0.59
2:B:802:PRO:HD2	2:B:805:VAL:HG21	1.85	0.59
1:A:673:GLN:HG2	1:A:685:LEU:HD12	1.84	0.59
2:B:751:LEU:HA	2:B:761:LEU:HD23	1.85	0.59
1:A:303:GLY:HA3	5:A:823:HOH:O	2.02	0.59
2:B:340:PRO:HB2	2:B:341:PHE:CD1	2.36	0.59
2:B:889:GLN:HG2	2:B:891:LEU:CD2	2.32	0.59
2:B:909:CYS:O	2:B:1007:GLU:HB2	2.02	0.59
1:A:155:LEU:HD12	1:A:158:LEU:HD12	1.83	0.59
2:B:321:PRO:HG2	2:B:734:HIS:HE1	1.68	0.59
2:B:529:ASN:ND2	2:B:531:GLN:H	2.01	0.59
2:B:469:MET:CE	2:B:678:LEU:HG	2.32	0.59
1:A:386:PHE:O	1:A:389:VAL:HB	2.02	0.59
2:B:941:ILE:HG23	2:B:953:ILE:HD11	1.84	0.58
1:A:352:LEU:HA	5:A:843:HOH:O	2.02	0.58
1:A:745:ASP:O	1:A:747:VAL:N	2.36	0.58
2:B:838:ASP:OD1	2:B:841:LYS:HE3	2.03	0.58
2:B:901:THR:CB	2:B:970:GLN:HE21	2.16	0.58
1:A:412:ARG:HG3	1:A:413:GLU:OE2	2.03	0.58
1:A:305:GLU:HG3	5:A:823:HOH:O	2.03	0.58
1:A:138:CYS:HB2	1:A:262:ARG:HH11	1.68	0.58
2:B:526:PHE:O	2:B:527:LEU:HB2	2.04	0.58
1:A:153:MET:SD	1:A:387:GLN:HB3	2.44	0.58
2:B:948:PRO:HG2	2:B:952:HIS:CE1	2.38	0.58
1:A:148:LYS:HE3	1:A:244:LEU:O	2.03	0.58
1:A:364:PRO:O	1:A:367:THR:O	2.22	0.58
2:B:492:ASN:C	2:B:494:VAL:H	2.05	0.58
2:B:852:LYS:HE2	2:B:1008:ASP:O	2.04	0.58
1:A:15:ASP:OD1	1:A:116:SER:HB2	2.04	0.58
2:B:633:VAL:HG11	2:B:651:VAL:HG12	1.86	0.58
1:A:407:GLU:HG3	1:A:445:GLN:HG3	1.85	0.57
2:B:492:ASN:OD1	2:B:492:ASN:O	2.22	0.57
1:A:536:THR:HG22	1:A:537:GLU:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:409:ARG:HG3	2:B:411:ASP:HB2	1.85	0.57
2:B:616:THR:HG22	2:B:617:ASN:N	2.20	0.57
2:B:296:VAL:HG12	2:B:314:ARG:NE	2.20	0.57
2:B:859:ARG:HB3	2:B:860:PRO:HD3	1.87	0.57
1:A:297:GLY:H	1:A:300:MET:CE	2.18	0.57
2:B:652:PRO:HA	2:B:655:THR:CG2	2.33	0.57
2:B:529:ASN:HD22	2:B:529:ASN:C	2.06	0.57
1:A:147:LEU:HD11	1:A:289:PHE:CD2	2.40	0.57
2:B:922:LEU:C	2:B:922:LEU:HD23	2.25	0.57
1:A:183:ILE:HD11	2:B:509:MET:HB2	1.86	0.56
1:A:652:THR:HG22	1:A:655:GLN:O	2.05	0.56
2:B:404:ASP:OD2	2:B:410:LEU:HB2	2.05	0.56
2:B:633:VAL:CG1	2:B:655:THR:HG21	2.35	0.56
2:B:898:VAL:HG22	2:B:967:TYR:CE2	2.40	0.56
2:B:962:GLU:HG2	2:B:963:VAL:N	2.19	0.56
2:B:608:GLU:OE1	2:B:803:LEU:HG	2.05	0.56
1:A:255:PRO:HG2	1:A:258:LYS:HG3	1.85	0.56
2:B:286:THR:OG1	2:B:304:ASP:O	2.20	0.56
2:B:332:ILE:HD12	2:B:777:LEU:HD13	1.88	0.56
2:B:446:MET:HE3	2:B:561:VAL:HG12	1.88	0.56
2:B:553:GLU:OE1	2:B:553:GLU:HA	2.05	0.56
2:B:962:GLU:HG2	2:B:963:VAL:H	1.70	0.56
1:A:536:THR:HG22	1:A:537:GLU:H	1.70	0.56
2:B:934:VAL:HG23	2:B:935:SER:H	1.70	0.56
2:B:945:PHE:HE2	2:B:990:ILE:HD13	1.70	0.56
1:A:426:LEU:HD12	1:A:445:GLN:HB3	1.88	0.56
1:A:418:GLY:HA3	1:A:438:ILE:O	2.06	0.56
2:B:1015:SER:HB2	2:B:1019:ASP:CB	2.35	0.56
1:A:349:ALA:HB1	1:A:355:THR:HG21	1.87	0.55
1:A:28:ARG:HH22	1:A:436:ASN:HD21	1.54	0.55
2:B:2:MET:HG2	2:B:1017:TYR:OH	2.06	0.55
2:B:601:LYS:CB	2:B:605:THR:HG21	2.28	0.55
2:B:775:ALA:O	2:B:779:LYS:HG3	2.07	0.55
2:B:902:MET:O	2:B:902:MET:HG2	2.05	0.55
2:B:562:ILE:HB	2:B:622:LEU:HD21	1.88	0.55
1:A:700:PHE:O	1:A:701:PRO:C	2.43	0.55
2:B:276:ARG:HA	2:B:298:THR:HG23	1.88	0.55
2:B:492:ASN:O	2:B:493:LYS:HG2	2.06	0.55
2:B:345:PRO:HD2	2:B:348:GLU:OE1	2.06	0.55
1:A:190:ARG:NH1	2:B:519:PHE:HB3	2.22	0.55
1:A:339:ALA:O	1:A:447:LYS:HE3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:845:VAL:HG22	2:B:1017:TYR:CE1	2.42	0.55
2:B:854:CYS:HB3	2:B:862:ILE:HD13	1.88	0.55
2:B:633:VAL:H	2:B:655:THR:CG2	2.17	0.55
1:A:171:ARG:HD2	5:A:826:HOH:O	2.06	0.55
2:B:585:LEU:HD21	2:B:594:LEU:CB	2.37	0.55
1:A:609:ARG:HG3	1:A:609:ARG:NH1	2.21	0.54
2:B:374:PHE:CE2	2:B:765:ASN:HB3	2.42	0.54
1:A:116:SER:HB2	1:A:497:THR:HG23	1.88	0.54
1:A:117:ILE:HG12	1:A:118:GLU:N	2.22	0.54
2:B:901:THR:CG2	2:B:902:MET:H	2.15	0.54
2:B:992:LYS:HB2	2:B:996:GLN:HG3	1.88	0.54
1:A:160:PRO:HB3	1:A:234:GLN:HB3	1.89	0.54
2:B:269:ILE:CD1	2:B:908:ARG:N	2.70	0.54
2:B:993:GLN:HG2	2:B:994:ARG:H	1.71	0.54
2:B:1025:HIS:ND1	3:C:192:MET:HG3	2.23	0.54
2:B:486:VAL:HG12	2:B:487:GLY:N	2.21	0.54
2:B:992:LYS:CD	2:B:996:GLN:HE21	2.19	0.54
2:B:356:HIS:CD2	2:B:362:VAL:H	2.21	0.54
1:A:95:PRO:HG2	1:A:98:TYR:CD1	2.43	0.54
2:B:469:MET:HE2	2:B:678:LEU:HG	1.88	0.54
2:B:469:MET:HE1	2:B:679:ARG:N	2.23	0.54
1:A:77:ASP:OD2	1:A:80:ALA:HB3	2.07	0.54
1:A:577:TYR:HB3	1:A:578:PRO:HD3	1.89	0.54
2:B:333:PRO:HD3	2:B:813:GLN:NE2	2.22	0.54
2:B:845:VAL:HG22	2:B:1017:TYR:CZ	2.43	0.54
2:B:854:CYS:HB2	2:B:862:ILE:HG21	1.89	0.54
2:B:964:GLY:HA3	2:B:968:SER:HB3	1.90	0.54
1:A:755:HIS:CD2	1:A:758:LYS:HE2	2.44	0.53
2:B:616:THR:HB	2:B:618:VAL:HG22	1.91	0.53
1:A:3:THR:HG22	1:A:5:LEU:N	2.20	0.53
1:A:297:GLY:H	1:A:300:MET:HE3	1.73	0.53
2:B:693:ARG:HG3	2:B:693:ARG:HH11	1.72	0.53
2:B:641:GLN:HG2	2:B:642:TYR:N	2.24	0.53
2:B:834:LEU:HD21	2:B:836:LEU:HD21	1.90	0.53
2:B:860:PRO:O	2:B:861:GLU:HB2	2.09	0.53
2:B:1030:GLN:C	2:B:1032:LEU:N	2.61	0.53
1:A:312:SER:H	1:A:315:ASP:HB2	1.73	0.53
2:B:267:SER:HB3	2:B:908:ARG:NH2	2.21	0.53
1:A:57:GLU:HG3	1:A:58:PRO:HD2	1.91	0.53
2:B:602:LEU:HA	2:B:608:GLU:HB2	1.90	0.53
2:B:852:LYS:O	2:B:857:LEU:HD22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:355:ASN:HD22	2:B:355:ASN:C	2.12	0.53
1:A:745:ASP:O	1:A:747:VAL:HG23	2.08	0.53
2:B:641:GLN:O	2:B:643:VAL:HG23	2.09	0.53
2:B:738:LEU:HB2	2:B:770:CYS:SG	2.49	0.53
2:B:446:MET:HE2	2:B:578:LEU:HB3	1.91	0.52
1:A:297:GLY:HA3	1:A:300:MET:HB2	1.90	0.52
2:B:288:THR:HG22	2:B:289:ARG:N	2.24	0.52
2:B:820:CYS:HA	2:B:823:LYS:HE2	1.91	0.52
2:B:965:ASN:HB3	2:B:966:PRO:HD3	1.90	0.52
2:B:589:GLU:O	2:B:590:ALA:HB2	2.10	0.52
2:B:996:GLN:CB	2:B:997:PRO:HD2	2.30	0.52
1:A:173:VAL:HG11	1:A:270:ILE:HD12	1.92	0.52
2:B:602:LEU:HD21	2:B:859:ARG:HD3	1.92	0.52
2:B:633:VAL:CG1	2:B:651:VAL:HG12	2.39	0.52
1:A:668:ARG:HA	1:A:673:GLN:NE2	2.25	0.52
2:B:661:LYS:NZ	2:B:661:LYS:HB3	2.25	0.52
1:A:397:GLN:NE2	1:A:489:SER:HB3	2.26	0.51
1:A:607:PHE:HD2	1:A:608:MET:HE3	1.74	0.51
2:B:446:MET:HE3	2:B:580:ILE:HG12	1.91	0.51
2:B:898:VAL:HG22	2:B:967:TYR:HE2	1.75	0.51
2:B:526:PHE:O	2:B:527:LEU:CB	2.59	0.51
1:A:195:LEU:HD22	1:A:203:MET:CE	2.41	0.51
1:A:317:ASP:C	1:A:319:ASP:H	2.12	0.51
2:B:605:THR:C	2:B:607:LYS:H	2.14	0.51
2:B:627:VAL:HG21	2:B:710:LEU:CD2	2.39	0.51
2:B:739:SER:C	2:B:741:ASP:H	2.14	0.51
2:B:1015:SER:HB2	2:B:1019:ASP:HB2	1.93	0.51
1:A:414:ILE:HG22	1:A:415:LYS:N	2.25	0.51
2:B:409:ARG:O	2:B:411:ASP:N	2.44	0.51
2:B:941:ILE:HD13	2:B:950:PHE:HA	1.93	0.51
1:A:696:LEU:HD12	1:A:703:PRO:HG2	1.93	0.51
1:A:259:ARG:HG3	1:A:306:LEU:HD23	1.91	0.51
1:A:79:ARG:HG3	1:A:79:ARG:HH11	1.76	0.50
1:A:547:ASP:HB3	1:A:743:LEU:HB2	1.93	0.50
2:B:269:ILE:HD11	2:B:908:ARG:N	2.26	0.50
2:B:523:LEU:HD23	5:B:1081:HOH:O	2.09	0.50
2:B:838:ASP:HA	2:B:841:LYS:HG3	1.93	0.50
2:B:937:PRO:HG2	2:B:940:LEU:HD12	1.92	0.50
2:B:641:GLN:HG2	2:B:642:TYR:H	1.77	0.50
1:A:662:GLU:HG3	1:A:710:HIS:CD2	2.46	0.50
2:B:372:CYS:HB2	2:B:373:PRO:CD	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLU:O	1:A:10:GLN:HG3	2.12	0.50
1:A:456:THR:O	1:A:528:ARG:NH2	2.43	0.50
1:A:656:ILE:HG13	1:A:695:ILE:CG2	2.41	0.50
1:A:528:ARG:HG3	1:A:608:MET:CE	2.41	0.50
2:B:267:SER:CB	2:B:908:ARG:HH21	2.23	0.50
1:A:138:CYS:HB2	1:A:262:ARG:NH1	2.26	0.50
2:B:317:THR:HG21	2:B:777:LEU:HD23	1.94	0.50
2:B:686:ILE:HG22	2:B:723:ASP:HB3	1.93	0.50
1:A:183:ILE:HD12	2:B:547:MET:CE	2.41	0.49
1:A:208:LYS:O	1:A:209:VAL:HB	2.12	0.49
1:A:392:LYS:HD3	1:A:396:GLY:HA2	1.94	0.49
1:A:536:THR:C	1:A:538:GLU:H	2.16	0.49
1:A:696:LEU:CD1	1:A:703:PRO:HG2	2.42	0.49
2:B:410:LEU:O	2:B:410:LEU:HG	2.11	0.49
2:B:544:ILE:HB	2:B:545:PRO:HD3	1.94	0.49
2:B:1025:HIS:CG	3:C:192:MET:HG3	2.47	0.49
1:A:53:PRO:O	1:A:54:ILE:O	2.30	0.49
2:B:469:MET:HE2	2:B:682:ILE:HD12	1.94	0.49
2:B:643:VAL:HG12	2:B:643:VAL:O	2.12	0.49
2:B:893:ILE:O	2:B:896:LEU:HB2	2.12	0.49
1:A:179:GLY:O	1:A:181:GLU:HG3	2.12	0.49
1:A:673:GLN:HG2	1:A:685:LEU:CD1	2.42	0.49
2:B:703:THR:HG21	2:B:733:LYS:HB2	1.95	0.49
2:B:775:ALA:HB1	2:B:779:LYS:HE3	1.95	0.49
2:B:618:VAL:HG23	2:B:619:TYR:N	2.27	0.49
2:B:813:GLN:O	2:B:817:MET:HG3	2.12	0.49
2:B:304:ASP:O	2:B:305:GLN:CB	2.61	0.49
2:B:974:ILE:CA	2:B:977:ILE:HG22	2.41	0.49
1:A:162:ALA:O	1:A:233:VAL:HG23	2.13	0.49
1:A:406:LEU:O	1:A:445:GLN:HA	2.13	0.49
1:A:536:THR:O	1:A:538:GLU:N	2.45	0.49
1:A:747:VAL:CG1	1:A:748:SER:H	2.08	0.49
2:B:898:VAL:O	2:B:899:LYS:C	2.51	0.49
1:A:15:ASP:HB3	1:A:497:THR:CG2	2.43	0.48
2:B:375:MET:SD	2:B:386:CYS:HA	2.52	0.48
1:A:511:GLN:H	1:A:511:GLN:NE2	2.11	0.48
2:B:534:GLN:HG2	2:B:538:HIS:CD2	2.48	0.48
1:A:596:SER:HG	1:A:599:GLU:HG3	1.79	0.48
2:B:1:ALA:N	3:C:190:ILE:HG23	2.29	0.48
2:B:992:LYS:CB	2:B:996:GLN:HG3	2.43	0.48
1:A:78:TYR:CD2	1:A:101:ILE:HG12	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:ARG:HH11	1:A:609:ARG:CG	2.20	0.48
1:A:744:THR:HG21	1:A:752:PHE:HD1	1.78	0.48
2:B:372:CYS:HA	2:B:417:GLU:O	2.13	0.48
2:B:942:GLN:CG	2:B:948:PRO:HA	2.43	0.48
2:B:979:GLN:HE22	2:B:986:MET:N	2.10	0.48
2:B:485:ARG:NH2	5:B:1083:HOH:O	2.41	0.48
2:B:529:ASN:ND2	2:B:529:ASN:C	2.66	0.48
2:B:955:THR:HG23	2:B:990:ILE:O	2.13	0.48
1:A:252:TRP:HB3	5:A:826:HOH:O	2.12	0.48
1:A:609:ARG:NH1	5:A:771:HOH:O	2.47	0.48
2:B:607:LYS:HG2	2:B:610:ILE:HD12	1.95	0.48
2:B:289:ARG:HD3	2:B:768:LEU:O	2.14	0.48
2:B:528:VAL:HG12	2:B:529:ASN:H	1.78	0.48
2:B:602:LEU:N	2:B:605:THR:OG1	2.46	0.48
2:B:854:CYS:CB	2:B:862:ILE:HD13	2.44	0.48
1:A:58:PRO:O	1:A:59:VAL:HB	2.13	0.48
1:A:509:GLN:O	1:A:510:ILE:C	2.52	0.48
2:B:2:MET:HE1	2:B:836:LEU:CD1	2.21	0.48
2:B:334:LEU:N	2:B:334:LEU:HD22	2.29	0.48
1:A:195:LEU:HD22	1:A:203:MET:HE2	1.95	0.47
2:B:693:ARG:HG3	2:B:693:ARG:NH1	2.27	0.47
2:B:289:ARG:O	2:B:291:GLN:N	2.45	0.47
2:B:766:LEU:HD21	2:B:768:LEU:HD21	1.96	0.47
1:A:314:HIS:HB3	1:A:318:LYS:HE3	1.96	0.47
2:B:279:ARG:NH2	2:B:293:PRO:C	2.68	0.47
2:B:356:HIS:CD2	2:B:361:PRO:HA	2.49	0.47
1:A:357:LEU:HD11	1:A:373:MET:HG3	1.95	0.47
2:B:649:GLY:O	2:B:652:PRO:HG2	2.14	0.47
1:A:19:PHE:CD2	1:A:40:ALA:HB2	2.50	0.47
1:A:143:ASP:OD2	1:A:376:SER:HB2	2.15	0.47
1:A:178:LEU:C	1:A:180:CYS:H	2.19	0.47
2:B:515:VAL:CG1	2:B:560:PRO:HG2	2.45	0.47
2:B:534:GLN:HG2	2:B:538:HIS:HD2	1.80	0.47
2:B:842:VAL:O	2:B:842:VAL:CG1	2.62	0.47
2:B:559:ALA:HB3	2:B:560:PRO:HD3	1.97	0.47
2:B:1025:HIS:O	2:B:1028:ILE:HG22	2.15	0.47
1:A:345:ILE:O	1:A:369:GLY:HA3	2.15	0.47
1:A:539:GLY:O	1:A:542:VAL:HG23	2.15	0.47
2:B:979:GLN:NE2	2:B:985:SER:HA	2.30	0.47
2:B:807:ARG:HG2	2:B:807:ARG:NH1	2.29	0.47
1:A:370:TYR:HA	5:A:813:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:TRP:O	1:A:549:GLN:HG2	2.15	0.46
2:B:529:ASN:HD21	2:B:531:GLN:HG2	1.80	0.46
1:A:313:TRP:CE2	1:A:597:PRO:HA	2.50	0.46
2:B:639:PRO:HB3	2:B:643:VAL:CG2	2.28	0.46
2:B:652:PRO:CA	2:B:655:THR:HG22	2.41	0.46
2:B:971:LEU:O	2:B:974:ILE:HG12	2.15	0.46
2:B:994:ARG:O	2:B:996:GLN:HG2	2.16	0.46
1:A:198:LYS:O	1:A:202:GLU:HG3	2.15	0.46
1:A:625:ALA:HB1	1:A:646:ARG:HG2	1.97	0.46
2:B:543:GLN:HB3	2:B:547:MET:HE1	1.97	0.46
2:B:319:CYS:HA	2:B:769:ASN:O	2.15	0.46
2:B:446:MET:CE	2:B:561:VAL:HG12	2.45	0.46
1:A:190:ARG:HB3	1:A:192:THR:HG22	1.98	0.46
2:B:996:GLN:CB	2:B:997:PRO:CD	2.90	0.46
2:B:312:PHE:CE1	2:B:344:ILE:HD11	2.50	0.46
2:B:888:PRO:HB3	2:B:922:LEU:HD21	1.97	0.46
1:A:39:ALA:HB3	1:A:525:LEU:HD13	1.98	0.46
2:B:559:ALA:N	2:B:560:PRO:CD	2.79	0.46
2:B:901:THR:HG22	2:B:903:LEU:H	1.80	0.46
2:B:739:SER:C	2:B:741:ASP:N	2.69	0.46
2:B:949:SER:O	2:B:952:HIS:HB2	2.16	0.46
2:B:395:VAL:HG11	2:B:400:PHE:HA	1.97	0.46
1:A:439:GLY:HA2	1:A:532:TYR:CE2	2.51	0.45
2:B:486:VAL:O	2:B:527:LEU:HA	2.16	0.45
2:B:499:ASN:HB3	2:B:508:GLN:HB2	1.98	0.45
2:B:1020:PHE:O	2:B:1024:VAL:HG23	2.16	0.45
1:A:275:LEU:HB3	1:A:343:HIS:CE1	2.51	0.45
1:A:350:CYS:HB2	1:A:377:PHE:CE1	2.51	0.45
2:B:402:HIS:O	2:B:409:ARG:HA	2.15	0.45
2:B:500:VAL:HG11	2:B:537:ILE:HG13	1.97	0.45
2:B:795:PHE:HB3	2:B:875:MET:HE2	1.98	0.45
1:A:491:GLN:HG2	1:A:493:ARG:HE	1.80	0.45
2:B:411:ASP:O	2:B:412:HIS:C	2.54	0.45
2:B:857:LEU:HD12	2:B:857:LEU:HA	1.69	0.45
1:A:196:SER:OG	1:A:199:GLN:HG3	2.17	0.45
1:A:505:ASP:O	1:A:509:GLN:N	2.50	0.45
1:A:638:ASP:OD1	1:A:639:SER:N	2.50	0.45
2:B:2:MET:CG	2:B:3:GLY:N	2.79	0.45
2:B:303:GLN:O	2:B:304:ASP:O	2.34	0.45
1:A:153:MET:CE	1:A:157:LEU:HD12	2.46	0.45
1:A:244:LEU:O	1:A:247:LEU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:GLN:O	1:A:511:GLN:N	2.50	0.45
2:B:469:MET:CE	2:B:679:ARG:HA	2.47	0.45
2:B:751:LEU:HD13	2:B:761:LEU:HD21	1.99	0.45
1:A:18:ARG:CZ	1:A:612:LEU:HD22	2.46	0.45
1:A:60:LEU:HB2	1:A:67:ARG:NH1	2.32	0.45
1:A:511:GLN:CD	1:A:511:GLN:N	2.67	0.45
1:A:660:HIS:HB2	1:A:709:GLU:HB3	1.98	0.45
2:B:599:ASP:HB3	2:B:601:LYS:HG3	1.98	0.45
2:B:643:VAL:CG1	2:B:648:LEU:HD12	2.46	0.45
2:B:834:LEU:HB2	2:B:1025:HIS:CD2	2.51	0.45
1:A:174:GLN:HG2	1:A:188:VAL:HG22	1.99	0.45
1:A:357:LEU:CD1	1:A:373:MET:HG3	2.47	0.45
2:B:515:VAL:HG13	2:B:560:PRO:CG	2.46	0.45
2:B:333:PRO:HD3	2:B:813:GLN:HE21	1.81	0.45
2:B:492:ASN:C	2:B:494:VAL:N	2.70	0.45
2:B:692:MET:HB2	2:B:750:VAL:HG22	1.98	0.45
1:A:252:TRP:HA	1:A:253:PRO:HD3	1.81	0.45
2:B:922:LEU:HD23	2:B:923:ALA:N	2.31	0.45
2:B:1015:SER:HB2	2:B:1019:ASP:HB3	1.99	0.45
2:B:407:GLY:C	2:B:409:ARG:N	2.71	0.44
2:B:455:LYS:C	2:B:457:GLY:H	2.19	0.44
2:B:624:LYS:HE2	2:B:624:LYS:HB3	1.81	0.44
1:A:296:GLN:CA	1:A:300:MET:HE2	2.40	0.44
1:A:153:MET:HE3	1:A:157:LEU:CD1	2.47	0.44
1:A:407:GLU:HA	1:A:444:CYS:O	2.17	0.44
1:A:609:ARG:NH1	1:A:609:ARG:CG	2.78	0.44
1:A:647:ILE:HD11	1:A:685:LEU:HD23	2.00	0.44
2:B:356:HIS:HE1	2:B:417:GLU:OE2	2.00	0.44
2:B:798:VAL:HG22	2:B:803:LEU:HD22	2.00	0.44
2:B:928:MET:O	2:B:988:LEU:HD12	2.17	0.44
1:A:618:MET:HE2	1:A:653:PHE:CD2	2.52	0.44
2:B:485:ARG:HB3	2:B:528:VAL:O	2.18	0.44
1:A:34:MET:O	1:A:36:VAL:N	2.47	0.44
2:B:476:GLU:HB3	2:B:478:GLN:HG3	2.00	0.44
2:B:603:VAL:HG12	2:B:604:ASN:ND2	2.32	0.44
2:B:605:THR:HG22	2:B:607:LYS:CB	2.48	0.44
2:B:891:LEU:HD12	2:B:904:PRO:O	2.17	0.44
2:B:899:LYS:O	2:B:900:SER:HB3	2.18	0.44
1:A:83:TRP:CE2	1:A:92:ASN:HB2	2.53	0.44
1:A:147:LEU:HD13	1:A:377:PHE:CD2	2.52	0.44
1:A:153:MET:HE1	1:A:154:SER:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:MET:SD	1:A:394:MET:N	2.87	0.44
1:A:582:PHE:O	1:A:586:ARG:HG2	2.18	0.44
1:A:417:SER:HB3	1:A:438:ILE:HG13	2.00	0.43
1:A:649:LEU:C	1:A:649:LEU:HD13	2.38	0.43
2:B:458:LEU:HD21	2:B:638:PHE:CG	2.53	0.43
2:B:993:GLN:O	2:B:994:ARG:C	2.57	0.43
1:A:747:VAL:HG11	1:A:751:VAL:HG11	2.00	0.43
2:B:312:PHE:HZ	2:B:344:ILE:HD11	1.79	0.43
2:B:535:SER:O	2:B:539:ASN:HB2	2.19	0.43
2:B:713:ASN:HD22	2:B:714:THR:N	2.16	0.43
2:B:970:GLN:NE2	2:B:973:MET:SD	2.91	0.43
2:B:800:HIS:C	2:B:801:GLN:HG3	2.38	0.43
2:B:814:THR:HA	2:B:817:MET:HE2	1.99	0.43
2:B:869:TYR:CE2	2:B:873:LEU:HD11	2.53	0.43
2:B:962:GLU:CG	2:B:963:VAL:H	2.28	0.43
1:A:461:PHE:CE2	1:A:479:ILE:HD13	2.54	0.43
2:B:2:MET:HG3	2:B:3:GLY:N	2.32	0.43
2:B:570:LYS:HE2	2:B:629:HIS:CE1	2.53	0.43
2:B:945:PHE:CD1	2:B:945:PHE:N	2.87	0.43
1:A:203:MET:HA	2:B:513:THR:HG21	2.01	0.43
1:A:319:ASP:OD1	1:A:319:ASP:O	2.36	0.43
1:A:693:GLN:O	1:A:697:HIS:CD2	2.71	0.43
2:B:469:MET:HE1	2:B:678:LEU:HG	1.99	0.43
1:A:236:ILE:O	1:A:237:ASP:C	2.57	0.43
1:A:311:ARG:HD2	5:A:833:HOH:O	2.19	0.43
1:A:652:THR:HG21	1:A:655:GLN:CG	2.47	0.43
1:A:695:ILE:C	1:A:697:HIS:H	2.22	0.43
2:B:609:LYS:O	2:B:613:GLN:HG3	2.19	0.43
2:B:837:PRO:HG2	2:B:840:MET:HB2	2.00	0.43
2:B:876:THR:CG2	5:B:1085:HOH:O	2.67	0.43
1:A:415:LYS:HB3	1:A:434:SER:HB2	2.01	0.43
1:A:618:MET:CE	1:A:653:PHE:CD2	3.02	0.43
2:B:453:ASN:O	2:B:459:VAL:HG23	2.19	0.43
2:B:993:GLN:CG	2:B:994:ARG:N	2.73	0.43
2:B:695:ARG:HG3	2:B:695:ARG:HH11	1.84	0.43
1:A:647:ILE:HG21	1:A:688:PRO:HG3	2.01	0.43
2:B:515:VAL:HG12	2:B:590:ALA:HB1	2.01	0.43
2:B:901:THR:HB	2:B:970:GLN:NE2	2.28	0.43
1:A:34:MET:C	1:A:35:VAL:CG1	2.87	0.42
1:A:359:GLU:OE1	1:A:359:GLU:N	2.48	0.42
1:A:651:ASP:OD1	1:A:652:THR:O	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:354:VAL:CG2	2:B:416:PRO:HG2	2.49	0.42
2:B:692:MET:HE1	2:B:728:VAL:CG1	2.45	0.42
2:B:955:THR:O	2:B:957:MET:N	2.52	0.42
1:A:28:ARG:HH22	1:A:436:ASN:ND2	2.17	0.42
1:A:505:ASP:H	1:A:509:GLN:HG3	1.84	0.42
2:B:540:LEU:O	2:B:544:ILE:HG13	2.19	0.42
2:B:713:ASN:HD22	2:B:715:THR:N	1.99	0.42
2:B:907:VAL:HG11	2:B:913:ARG:HB3	2.01	0.42
1:A:748:SER:OG	1:A:751:VAL:HG23	2.19	0.42
2:B:430:ASP:OD2	2:B:430:ASP:N	2.46	0.42
2:B:1000:VAL:HA	2:B:1003:GLN:NE2	2.27	0.42
1:A:70:LEU:HD13	1:A:83:TRP:CD2	2.55	0.42
1:A:564:ASP:O	1:A:565:PRO:C	2.57	0.42
2:B:326:MET:O	2:B:329:GLN:HB2	2.20	0.42
2:B:486:VAL:CG1	2:B:487:GLY:N	2.82	0.42
2:B:577:LYS:HA	2:B:632:SER:O	2.18	0.42
1:A:153:MET:HE3	1:A:157:LEU:HD12	2.01	0.42
2:B:304:ASP:O	2:B:305:GLN:HB2	2.19	0.42
2:B:907:VAL:CG1	2:B:913:ARG:HB3	2.49	0.42
1:A:526:MET:HG3	1:A:577:TYR:OH	2.19	0.42
2:B:356:HIS:CD2	2:B:362:VAL:HG23	2.55	0.42
2:B:934:VAL:CG2	2:B:935:SER:N	2.82	0.42
1:A:121:VAL:HG12	1:A:123:ARG:N	2.35	0.42
1:A:268:LEU:HD23	1:A:268:LEU:HA	1.87	0.42
1:A:636:LEU:CG	1:A:638:ASP:HB2	2.48	0.42
1:A:669:LYS:HE3	1:A:709:GLU:OE2	2.20	0.42
1:A:743:LEU:O	1:A:755:HIS:ND1	2.52	0.42
2:B:361:PRO:O	2:B:363:ARG:HG3	2.20	0.42
2:B:600:LYS:CA	2:B:859:ARG:NH1	2.80	0.42
2:B:891:LEU:N	2:B:891:LEU:HD22	2.35	0.42
2:B:992:LYS:O	2:B:996:GLN:HB2	2.20	0.42
1:A:134:VAL:HG11	1:A:288:MET:HE3	2.01	0.42
1:A:208:LYS:O	1:A:209:VAL:CB	2.68	0.42
2:B:269:ILE:CD1	2:B:907:VAL:C	2.87	0.42
2:B:853:ASN:ND2	2:B:855:VAL:HB	2.34	0.42
1:A:147:LEU:HG	1:A:151:MET:CE	2.50	0.42
2:B:854:CYS:O	2:B:867:ARG:HD2	2.19	0.42
1:A:72:PRO:HD3	1:A:109:GLU:O	2.20	0.41
1:A:116:SER:CB	1:A:497:THR:HG23	2.50	0.41
2:B:616:THR:CG2	2:B:618:VAL:HG13	2.50	0.41
2:B:695:ARG:HG3	2:B:695:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:GLN:O	1:A:388:ARG:HG3	2.20	0.41
1:A:413:GLU:C	1:A:464:VAL:HG12	2.41	0.41
2:B:367:CYS:O	2:B:368:LYS:HB2	2.21	0.41
2:B:1027:GLU:O	2:B:1031:LEU:HG	2.21	0.41
2:B:1029:CYS:O	2:B:1032:LEU:HA	2.20	0.41
2:B:570:LYS:HE2	2:B:629:HIS:NE2	2.35	0.41
2:B:798:VAL:HG22	2:B:803:LEU:CD2	2.51	0.41
2:B:372:CYS:HB2	2:B:373:PRO:HD2	2.02	0.41
2:B:484:ILE:HD11	2:B:755:ILE:HB	2.02	0.41
2:B:861:GLU:O	2:B:862:ILE:O	2.39	0.41
2:B:1009:LYS:CG	2:B:1016:SER:HB3	2.51	0.41
1:A:236:ILE:CG2	1:A:240:LEU:HB2	2.47	0.41
2:B:974:ILE:HG13	2:B:975:MET:N	2.36	0.41
1:A:148:LYS:O	1:A:152:GLN:HG3	2.20	0.41
1:A:510:ILE:HB	1:A:511:GLN:NE2	2.36	0.41
1:A:536:THR:C	1:A:538:GLU:N	2.73	0.41
2:B:434:LYS:O	2:B:436:LYS:HG3	2.20	0.41
2:B:501:LYS:NZ	2:B:524:ASP:HB3	2.35	0.41
2:B:933:GLY:HA2	2:B:993:GLN:HB2	2.03	0.41
1:A:259:ARG:HG3	1:A:306:LEU:CD2	2.51	0.41
1:A:368:GLY:HA3	1:A:450:GLY:O	2.20	0.41
1:A:414:ILE:CG2	1:A:415:LYS:N	2.84	0.41
2:B:302:ILE:HD12	2:B:311:ARG:NE	2.36	0.41
2:B:661:LYS:HB3	2:B:661:LYS:HZ2	1.84	0.41
2:B:665:PHE:CE1	2:B:670:ASP:HB2	2.55	0.41
2:B:723:ASP:OD2	2:B:726:LYS:HE2	2.21	0.41
1:A:313:TRP:HA	1:A:316:ILE:CG2	2.51	0.41
2:B:515:VAL:HG13	2:B:560:PRO:HG2	2.02	0.41
2:B:571:ALA:C	2:B:573:ASP:H	2.23	0.41
1:A:15:ASP:HB3	1:A:497:THR:HG21	2.02	0.40
1:A:25:PRO:CG	1:A:31:ALA:HB2	2.51	0.40
1:A:172:MET:HE2	1:A:252:TRP:HE1	1.86	0.40
1:A:313:TRP:NE1	1:A:592:VAL:HB	2.36	0.40
2:B:605:THR:C	2:B:607:LYS:N	2.72	0.40
2:B:627:VAL:CG2	2:B:710:LEU:HD23	2.49	0.40
1:A:254:VAL:HA	1:A:255:PRO:HD2	1.83	0.40
1:A:313:TRP:NE1	1:A:597:PRO:HA	2.37	0.40
1:A:695:ILE:HG22	1:A:696:LEU:HD13	2.03	0.40
2:B:676:ASN:O	2:B:680:ASN:HB2	2.21	0.40
2:B:921:LEU:HD12	2:B:974:ILE:CD1	2.51	0.40
1:A:77:ASP:OD2	1:A:80:ALA:CB	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:366:LEU:HD23	1:A:366:LEU:HA	1.80	0.40
2:B:523:LEU:HD23	2:B:523:LEU:HA	1.82	0.40
2:B:605:THR:O	2:B:606:ASP:CB	2.70	0.40
1:A:548:ARG:HH21	1:A:549:GLN:HE22	1.69	0.40
2:B:465:GLU:HG2	2:B:675:LEU:CD2	2.45	0.40
2:B:982:ARG:HA	2:B:983:PRO:HD2	1.83	0.40
2:B:992:LYS:HB2	2:B:996:GLN:HE21	1.85	0.40
1:A:41:LEU:HD12	1:A:41:LEU:HA	1.95	0.40
1:A:747:VAL:HG11	1:A:751:VAL:CB	2.52	0.40
2:B:577:LYS:HE2	2:B:579:PHE:CZ	2.57	0.40
2:B:623:ALA:O	2:B:627:VAL:HG23	2.20	0.40
2:B:707:GLY:HA2	2:B:875:MET:O	2.21	0.40
2:B:955:THR:C	2:B:957:MET:H	2.25	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	708/765 (92%)	635 (90%)	54 (8%)	19 (3%)	4	10
2	B	763/770 (99%)	659 (86%)	75 (10%)	29 (4%)	2	6
3	C	5/7 (71%)	5 (100%)	0	0	100	100
All	All	1476/1542 (96%)	1299 (88%)	129 (9%)	48 (3%)	3	7

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	746	ASP
2	B	289	ARG
2	B	304	ASP

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Mol	Chain	Res	Type
2	B	408	ARG
2	B	412	HIS
2	B	492	ASN
2	B	900	SER
2	B	964	GLY
2	B	993	GLN
2	B	996	GLN
2	B	998	GLU
2	B	1032	LEU
1	A	54	ILE
1	A	80	ALA
1	A	180	CYS
1	A	237	ASP
1	A	537	GLU
1	A	593	PHE
2	B	410	LEU
2	B	527	LEU
2	B	862	ILE
2	B	899	LYS
2	B	902	MET
2	B	956	ASP
2	B	995	GLU
1	A	184	SER
1	A	540	PRO
1	A	700	PHE
1	A	744	THR
2	B	503	ASN
2	B	860	PRO
2	B	963	VAL
2	B	980	GLN
1	A	536	THR
1	A	696	LEU
2	B	903	LEU
2	B	966	PRO
1	A	59	VAL
1	A	99	ALA
2	B	397	PRO
2	B	994	ARG
1	A	324	VAL
1	A	510	ILE
2	B	290	GLY
2	B	590	ALA

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Mol	Chain	Res	Type
2	B	961	PRO
1	A	565	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	626/665 (94%)	595 (95%)	31 (5%)	20	46
2	B	680/682 (100%)	645 (95%)	35 (5%)	20	45
3	C	6/6 (100%)	6 (100%)	0	100	100
All	All	1312/1353 (97%)	1246 (95%)	66 (5%)	20	46

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	35	VAL
1	A	41	LEU
1	A	67	ARG
1	A	105	ASN
1	A	153	MET
1	A	194	ASP
1	A	237	ASP
1	A	240	LEU
1	A	243	LEU
1	A	268	LEU
1	A	301	VAL
1	A	308	THR
1	A	311	ARG
1	A	317	ASP
1	A	320	ASN
1	A	332	GLU
1	A	373	MET
1	A	394	MET
1	A	451	LEU

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Mol	Chain	Res	Type
1	A	491	GLN
1	A	528	ARG
1	A	565	PRO
1	A	570	PHE
1	A	609	ARG
1	A	637	LEU
1	A	673	GLN
1	A	677	GLU
1	A	690	ASP
1	A	695	ILE
1	A	696	LEU
2	B	305	GLN
2	B	355	ASN
2	B	356	HIS
2	B	376	GLN
2	B	391	CYS
2	B	401	GLN
2	B	408	ARG
2	B	409	ARG
2	B	411	ASP
2	B	470	LEU
2	B	475	LYS
2	B	478	GLN
2	B	485	ARG
2	B	523	LEU
2	B	529	ASN
2	B	553	GLU
2	B	566	MET
2	B	599	ASP
2	B	620	ASP
2	B	633	VAL
2	B	653	GLN
2	B	661	LYS
2	B	691	ILE
2	B	713	ASN
2	B	777	LEU
2	B	799	LEU
2	B	807	ARG
2	B	834	LEU
2	B	843	LEU
2	B	896	LEU
2	B	921	LEU

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Mol	Chain	Res	Type
2	B	946	ASN
2	B	958	THR
2	B	980	GLN
2	B	1027	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	227	ASN
1	A	239	ASN
1	A	320	ASN
1	A	397	GLN
1	A	436	ASN
1	A	486	GLN
1	A	511	GLN
1	A	549	GLN
1	A	579	GLN
1	A	591	GLN
1	A	595	ASN
1	A	620	GLN
1	A	673	GLN
1	A	697	HIS
1	A	710	HIS
2	B	355	ASN
2	B	356	HIS
2	B	385	GLN
2	B	492	ASN
2	B	503	ASN
2	B	506	GLN
2	B	508	GLN
2	B	529	ASN
2	B	613	GLN
2	B	615	GLN
2	B	617	ASN
2	B	666	GLN
2	B	668	HIS
2	B	713	ASN
2	B	773	GLN
2	B	813	GLN
2	B	816	HIS
2	B	824	ASN

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Mol	Chain	Res	Type
2	B	853	ASN
2	B	942	GLN
2	B	946	ASN
2	B	969	GLN
2	B	970	GLN
2	B	979	GLN
2	B	996	GLN
2	B	1003	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	716/765 (93%)	-0.09	23 (3%)	50 48	26, 53, 94, 131	0
2	B	767/770 (99%)	0.01	43 (5%)	31 29	26, 54, 109, 141	0
3	C	7/7 (100%)	0.26	1 (14%)	7 7	56, 60, 91, 119	0
All	All	1490/1542 (96%)	-0.04	67 (4%)	39 37	26, 54, 102, 141	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	540	PRO	6.8
2	B	960	LEU	5.2
2	B	1033	ASN	4.9
1	A	742	ILE	4.9
2	B	860	PRO	4.6
1	A	209	VAL	4.5
2	B	966	PRO	4.0
1	A	52	PRO	4.0
2	B	997	PRO	4.0
1	A	53	PRO	3.9
2	B	955	THR	3.9
1	A	741	PRO	3.8
2	B	2	MET	3.7
1	A	539	GLY	3.7
1	A	51	LEU	3.5
2	B	1010	GLY	3.4
2	B	3	GLY	3.4
2	B	857	LEU	3.3
2	B	963	VAL	3.3
2	B	1	ALA	3.1
2	B	959	LEU	3.0
2	B	901	THR	2.9
2	B	967	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	961	PRO	2.8
2	B	964	GLY	2.7
2	B	951	ALA	2.7
2	B	1028	ILE	2.7
2	B	947	VAL	2.6
2	B	965	ASN	2.6
1	A	510	ILE	2.6
1	A	314	HIS	2.6
2	B	601	LYS	2.5
2	B	410	LEU	2.5
2	B	406	ILE	2.5
2	B	957	MET	2.5
1	A	464	VAL	2.5
2	B	862	ILE	2.5
1	A	122	LEU	2.5
2	B	896	LEU	2.5
2	B	405	HIS	2.5
2	B	1032	LEU	2.4
1	A	762	SER	2.4
2	B	299	ASP	2.4
2	B	603	VAL	2.3
2	B	859	ARG	2.3
1	A	743	LEU	2.3
2	B	602	LEU	2.3
1	A	79	ARG	2.2
2	B	858	SER	2.2
1	A	536	THR	2.2
2	B	823	LYS	2.2
2	B	899	LYS	2.2
2	B	404	ASP	2.2
2	B	524	ASP	2.2
1	A	318	LYS	2.2
2	B	902	MET	2.1
1	A	544	ARG	2.1
1	A	701	PRO	2.1
2	B	551	SER	2.1
2	B	407	GLY	2.1
1	A	3	THR	2.1
3	C	193	MET	2.0
1	A	744	THR	2.0
1	A	698	SER	2.0
1	A	180	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	958	THR	2.0
2	B	528	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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( $\text{\AA}^2$ )	Q<0.9
4	ZN	A	766	1/1	1.00	0.04	46,46,46,46	0
4	ZN	B	1034	1/1	1.00	0.02	57,57,57,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.