



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 8, 2016 – 04:49 PM EDT

PDB ID : 5KYY  
Title : Crystal structure of Sec23 and TANGO1 peptide4 complex  
Authors : Ma, W.; Goldberg, J.  
Deposited on : 2016-07-22  
Resolution : 3.40 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : unknown  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

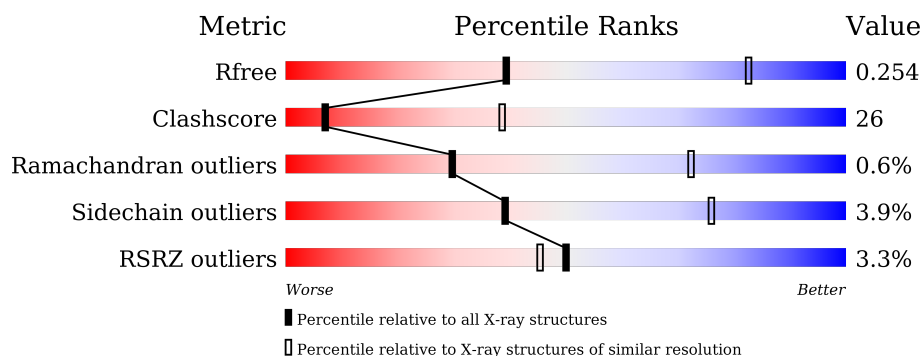
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1476 (3.50-3.30)
Clashscore	102246	1611 (3.50-3.30)
Ramachandran outliers	100387	1571 (3.50-3.30)
Sidechain outliers	100360	1571 (3.50-3.30)
RSRZ outliers	91569	1485 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>2%</div> <div> <div></div> <div>58%</div> <div>34%</div> <div>6%</div> </div> </div>
2	B	770	<div> <div>4%</div> <div> <div></div> <div>58%</div> <div>39%</div> <div>.</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ZN	A	801	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11682 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
			5676	3619	975	1042	40			

- Molecule 2 is a protein called Protein transport protein Sec24D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	767	Total	C	N	O	S	0	0	0
			6004	3822	1014	1114	54			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	ALA	-	expression tag	UNP O94855
B	2	MET	-	expression tag	UNP O94855
B	3	GLY	-	expression tag	UNP O94855

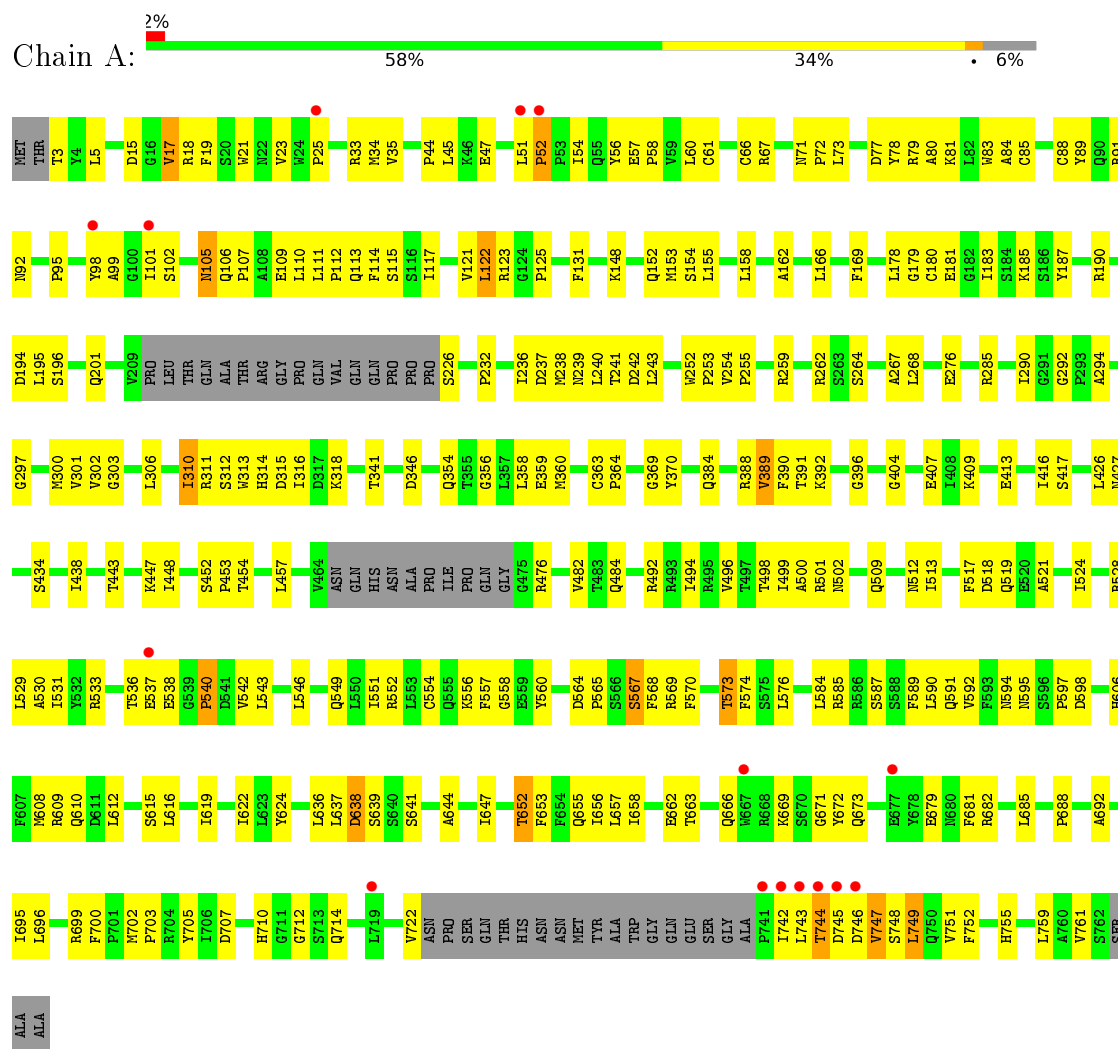
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

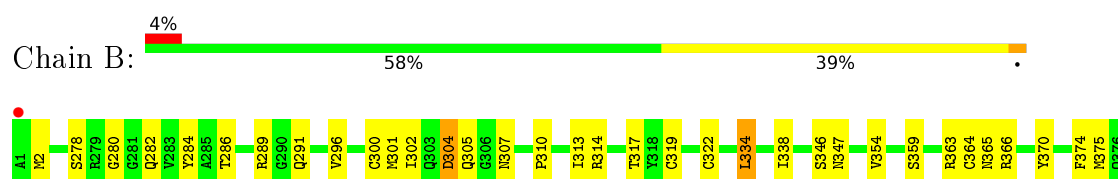
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: Protein transport protein Sec23A



#### • Molecule 2: Protein transport protein Sec24D



K1026	E1027	I1028	G1029	Q1030	L1031	L1032	M1033	I953	D956	M957	T958	L959	L960	P961	E962	V963	G964	N965	P966	Y967	S968	Q969	Q970	M973	I974	M975	G976	I977	I978	Q979	R982	S985	L988	K992	Q993	Q996	P997	E998	M999	V1000	F1001	R1002	K1009	G1010	LEU	TRR	GLY	G1014	S1015	S1016	Y1017	V1018	D1019	F1020	L1021	C1022	V1023	H1024	S1025	S858	R859	P860	E861	Q870	R871	Q872	M875	T876	Q889	I893	L896	K899	S900	T901	M902	L903	V907	R908	E911	S912	R913	L914	S915	E916	I919	F920	L921	L922	M928	W931	L932	G933	V934	S935	S936	I941	Q942	G943	I944	F945	N946	V947	P948	S949	F950	A951	H952	Q758	R759	R760	N765	L766	L767	L768	N769	C770	S771	L777	E782	L787	N788	F789	K792	F795	V798	P802	L803	L810	Q813	M817	L818	C820	Y821	R822	K823	N824	C825	A826	S829	A830	A831	S832	Q833	L834	I835	L836	P837	V845	Y846	C854	L857	L650	V651	F652	Q653	L654	T655	R661	N662	N663	N664	F674	L678	R679	L686	G687	R693	V694	R695	T696	S697	T698	T703	D704	L709	L710	D716	M719	D723	C724	D725	K726	E731	D735	D736	K737	L738	D741	S742	L745	V746	Q747	L751	G576	K577	L578	F579	S583	S584	L585	P586	T587	A588	E589	A590	P591	G592	L594	D599	K600	K601	L602	V603	N604	T605	D606	K607	E608	K609	I610	L611	F612	Q613	P614	N617	S621	K624	D625	C626	V627	A628	H629	S632	V633	L637	F638	P639	S640	Q641	Y642	V643	D644	V645	S647	K472	I473	E474	K475	Q478	L484	F488	C489	T490	Y491	M492	K493	H496	F497	F498	M499	V500	V515	G516	E517	V518	F519	V520	P521	L522	L523	D524	G525	F526	L527	V528	N529	Y530	S533	I537	L541	D542	Q543	N547	F548	N554	V557	P560	L569	K570	T568	M569	L570	E571
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.39Å 139.06Å 149.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.01 – 3.40 48.01 – 3.40	Depositor EDS
% Data completeness (in resolution range)	83.9 (48.01-3.40) 81.4 (48.01-3.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.20 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, $R_{free}$	0.177 , 0.253 0.198 , 0.254	Depositor DCC
$R_{free}$ test set	1919 reflections (7.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	82.4	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 53.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11682	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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	0.61	0/5809	0.73	0/7868
2	B	0.67	0/6132	0.76	0/8309
All	All	0.64	0/11941	0.75	0/16177

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

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	5676	0	5627	290	0
2	B	6004	0	5968	331	0
3	A	1	0	0	2	0
3	B	1	0	0	0	0
All	All	11682	0	11595	614	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 (614) 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:51:LEU:HD21	1:A:117:ILE:HA	1.43	0.96
2:B:967:TYR:O	2:B:969:GLN:N	1.99	0.96
1:A:652:THR:HG23	1:A:655:GLN:H	1.29	0.94
2:B:366:ARG:NH2	2:B:391:CYS:HB2	1.83	0.93
2:B:931:TRP:CZ2	2:B:993:GLN:HG3	2.04	0.93
1:A:673:GLN:N	1:A:673:GLN:OE1	2.01	0.92
1:A:311:ARG:HH21	1:A:311:ARG:HG3	1.33	0.92
2:B:896:LEU:HD21	2:B:970:GLN:CG	2.00	0.92
2:B:996:GLN:HB3	2:B:997:PRO:HD2	1.52	0.90
1:A:564:ASP:HB3	1:A:567:SER:HB3	1.54	0.90
2:B:492:ASN:O	2:B:492:ASN:OD1	1.90	0.88
2:B:703:THR:O	2:B:704:ASP:OD1	1.91	0.88
1:A:66:CYS:HG	3:A:801:ZN:ZN	0.84	0.88
2:B:822:ARG:O	2:B:826:ALA:HB3	1.74	0.87
2:B:861:GLU:HG3	2:B:861:GLU:O	1.73	0.86
2:B:586:PRO:HG2	2:B:594:LEU:HD12	1.57	0.86
2:B:492:ASN:O	2:B:493:LYS:HB3	1.75	0.86
2:B:601:LYS:C	2:B:605:THR:HG21	1.96	0.86
2:B:406:ILE:HG22	2:B:406:ILE:O	1.74	0.85
2:B:633:VAL:H	2:B:655:THR:HG21	1.42	0.85
2:B:934:VAL:N	2:B:993:GLN:OE1	2.10	0.85
2:B:617:ASN:ND2	2:B:617:ASN:O	2.09	0.85
1:A:35:VAL:HG21	1:A:552:ARG:HB3	1.58	0.84
1:A:564:ASP:O	1:A:567:SER:CB	2.25	0.84
2:B:932:LEU:O	2:B:993:GLN:HB2	1.77	0.84
2:B:1024:VAL:HG12	2:B:1028:ILE:HD11	1.58	0.83
1:A:749:LEU:O	1:A:749:LEU:HD12	1.77	0.83
2:B:500:VAL:HG11	2:B:537:ILE:HG12	1.62	0.82
1:A:35:VAL:HG13	1:A:549:GLN:NE2	1.94	0.81
1:A:673:GLN:O	1:A:682:ARG:CG	2.29	0.81
2:B:493:LYS:O	2:B:493:LYS:HG3	1.79	0.81
2:B:896:LEU:HD21	2:B:970:GLN:HG3	1.61	0.81
1:A:564:ASP:O	1:A:567:SER:HB3	1.81	0.81
2:B:998:GLU:O	2:B:1002:ARG:HG3	1.81	0.81
1:A:51:LEU:HD12	1:A:52:PRO:CD	2.11	0.81
2:B:384:TYR:CE1	2:B:393:ASN:HB2	2.15	0.81
1:A:179:GLY:CA	1:A:236:ILE:HD11	2.11	0.81
1:A:673:GLN:O	1:A:682:ARG:HG2	1.80	0.81
1:A:564:ASP:O	1:A:567:SER:N	2.13	0.80
2:B:747:GLN:NE2	2:B:765:ASN:OD1	2.14	0.80
2:B:590:ALA:HB1	2:B:591:PRO:CD	2.12	0.80
2:B:493:LYS:CG	2:B:493:LYS:O	2.30	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:944:ILE:HG22	2:B:945:PHE:CD1	2.17	0.79
2:B:490:THR:HG23	2:B:498:PHE:HE2	1.45	0.79
2:B:899:LYS:O	2:B:900:SER:OG	2.01	0.79
2:B:412:HIS:O	2:B:419:SER:HB3	1.83	0.78
2:B:470:LEU:HD12	2:B:530:TYR:CE1	2.19	0.78
2:B:590:ALA:HB1	2:B:591:PRO:HD2	1.66	0.78
1:A:551:ILE:HD11	1:A:743:LEU:HD13	1.66	0.78
1:A:57:GLU:HG3	1:A:58:PRO:HD2	1.65	0.78
2:B:792:LYS:HE2	2:B:875:MET:O	1.84	0.77
2:B:795:PHE:O	2:B:871:ARG:NH1	2.17	0.77
2:B:1024:VAL:O	2:B:1028:ILE:HG13	1.86	0.76
1:A:179:GLY:HA2	1:A:236:ILE:HD11	1.66	0.76
2:B:469:MET:HE3	2:B:679:ARG:N	2.01	0.75
2:B:896:LEU:HD21	2:B:970:GLN:HG2	1.68	0.75
2:B:591:PRO:CD	2:B:591:PRO:O	2.30	0.75
2:B:934:VAL:HG13	2:B:993:GLN:OE1	1.86	0.75
2:B:468:THR:HG22	2:B:469:MET:N	2.02	0.75
1:A:744:THR:HG23	1:A:745:ASP:O	1.87	0.74
1:A:636:LEU:HG	1:A:638:ASP:HB2	1.68	0.74
2:B:469:MET:HE3	2:B:679:ARG:HA	1.69	0.74
1:A:745:ASP:O	1:A:747:VAL:HG22	1.86	0.74
1:A:564:ASP:CB	1:A:567:SER:HB3	2.18	0.74
1:A:179:GLY:O	1:A:181:GLU:HG3	1.86	0.74
2:B:1024:VAL:HG12	2:B:1028:ILE:CD1	2.17	0.74
2:B:469:MET:CE	2:B:679:ARG:HA	2.17	0.74
1:A:388:ARG:O	1:A:390:PHE:N	2.22	0.73
1:A:15:ASP:OD1	1:A:115:SER:OG	2.06	0.73
1:A:264:SER:HB2	1:A:294:ALA:HB2	1.70	0.73
1:A:499:ILE:O	1:A:499:ILE:HD12	1.89	0.73
1:A:681:PHE:CE2	1:A:685:LEU:HD11	2.23	0.72
2:B:366:ARG:NH2	2:B:391:CYS:CB	2.52	0.72
2:B:469:MET:HE3	2:B:679:ARG:CA	2.20	0.72
2:B:979:GLN:NE2	2:B:985:SER:HA	2.04	0.72
2:B:466:LEU:O	2:B:467:LYS:C	2.24	0.72
1:A:71:ASN:HB3	1:A:498:THR:HG21	1.70	0.72
2:B:489:ILE:HD11	2:B:526:PHE:HZ	1.53	0.72
2:B:528:VAL:HG11	2:B:533:SER:OG	1.89	0.72
1:A:673:GLN:HB3	1:A:685:LEU:HD12	1.72	0.71
1:A:60:LEU:HB3	1:A:67:ARG:NH1	2.04	0.71
1:A:107:PRO:HD2	1:A:110:LEU:HD12	1.72	0.71
2:B:792:LYS:CE	2:B:875:MET:O	2.38	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:522:LEU:HD12	2:B:522:LEU:C	2.11	0.71
2:B:587:THR:O	2:B:593:LYS:HE3	1.89	0.71
1:A:51:LEU:CD1	1:A:114:PHE:CE1	2.74	0.71
1:A:237:ASP:O	1:A:241:THR:HG22	1.90	0.71
2:B:470:LEU:CD1	2:B:530:TYR:CE1	2.73	0.71
1:A:54:ILE:HG21	1:A:56:TYR:CE2	2.25	0.71
2:B:639:PRO:HB3	2:B:643:VAL:HG21	1.72	0.71
2:B:921:LEU:HD11	2:B:975:MET:HG2	1.73	0.70
1:A:51:LEU:CD2	1:A:117:ILE:HA	2.19	0.70
2:B:379:GLU:OE1	2:B:383:ARG:HD2	1.91	0.70
1:A:51:LEU:HD12	1:A:52:PRO:HD2	1.72	0.70
2:B:758:GLN:OE1	2:B:760:ARG:NH2	2.23	0.70
2:B:591:PRO:HD2	2:B:591:PRO:O	1.91	0.69
1:A:311:ARG:HE	1:A:359:GLU:CD	1.94	0.69
1:A:123:ARG:HG3	1:A:125:PRO:HD2	1.73	0.69
2:B:586:PRO:CG	2:B:594:LEU:HD12	2.23	0.68
1:A:509:GLN:HB3	1:A:512:ASN:HB2	1.74	0.68
1:A:657:LEU:C	1:A:657:LEU:HD23	2.14	0.68
1:A:743:LEU:CD1	1:A:759:LEU:HD12	2.23	0.68
2:B:518:VAL:HG12	2:B:519:PHE:N	2.08	0.68
2:B:607:LYS:HE2	2:B:610:ILE:HD12	1.75	0.68
1:A:302:VAL:HG22	1:A:303:GLY:N	2.07	0.68
1:A:652:THR:HG23	1:A:655:GLN:N	2.08	0.68
2:B:403:LEU:HB3	2:B:407:GLY:HA2	1.75	0.68
2:B:602:LEU:N	2:B:605:THR:HG21	2.09	0.68
1:A:311:ARG:NH2	1:A:311:ARG:HG3	2.09	0.68
1:A:35:VAL:HG13	1:A:549:GLN:HE21	1.59	0.68
1:A:61:CYS:SG	1:A:85:CYS:HB2	2.34	0.67
1:A:185:LYS:NZ	1:A:187:TYR:OH	2.26	0.67
2:B:942:GLN:O	2:B:946:ASN:HA	1.94	0.67
2:B:992:LYS:CB	2:B:996:GLN:HG3	2.25	0.67
1:A:238:MET:HE2	1:A:238:MET:HA	1.76	0.67
2:B:522:LEU:HD12	2:B:523:LEU:N	2.10	0.67
1:A:312:SER:HG	1:A:315:ASP:CG	1.97	0.67
2:B:366:ARG:CZ	2:B:391:CYS:HB2	2.24	0.67
2:B:464:GLU:OE2	2:B:467:LYS:NZ	2.26	0.67
2:B:697:SER:HB3	2:B:745:LEU:HB2	1.76	0.67
1:A:743:LEU:O	1:A:755:HIS:ND1	2.27	0.67
1:A:743:LEU:O	1:A:755:HIS:CE1	2.48	0.66
2:B:792:LYS:NZ	2:B:875:MET:O	2.28	0.66
1:A:531:ILE:HB	1:A:608:MET:HE1	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:TYR:HE2	1:A:389:VAL:HG13	1.60	0.66
2:B:958:THR:HG21	2:B:988:LEU:O	1.96	0.66
1:A:482:VAL:HG13	1:A:496:VAL:HG22	1.77	0.65
2:B:1027:GLU:HA	2:B:1030:GLN:HB2	1.79	0.65
2:B:406:ILE:CG2	2:B:406:ILE:O	2.43	0.65
2:B:641:GLN:O	2:B:643:VAL:HG23	1.97	0.65
2:B:859:ARG:O	2:B:860:PRO:C	2.30	0.65
2:B:377:PHE:CE2	2:B:409:ARG:HD2	2.31	0.65
2:B:304:ASP:O	2:B:305:GLN:HB2	1.96	0.65
1:A:499:ILE:HD12	1:A:499:ILE:C	2.18	0.65
2:B:820:CYS:HA	2:B:823:LYS:HE2	1.79	0.64
2:B:946:ASN:ND2	2:B:946:ASN:O	2.30	0.64
2:B:661:LYS:NZ	2:B:663:ASN:HD21	1.95	0.64
1:A:54:ILE:CG2	1:A:56:TYR:CE2	2.80	0.64
1:A:748:SER:OG	1:A:751:VAL:HG23	1.98	0.64
2:B:736:ASP:OD1	2:B:737:LYS:N	2.30	0.64
1:A:71:ASN:CB	1:A:498:THR:HG21	2.26	0.64
1:A:312:SER:OG	1:A:315:ASP:OD2	2.15	0.64
1:A:285:ARG:NH2	1:A:346:ASP:OD2	2.31	0.64
2:B:590:ALA:CB	2:B:591:PRO:HD2	2.28	0.63
1:A:102:SER:HB3	1:A:105:ASN:H	1.64	0.63
1:A:746:ASP:O	1:A:747:VAL:HG13	1.98	0.63
1:A:54:ILE:HG22	1:A:56:TYR:CD2	2.34	0.63
2:B:322:CYS:SG	2:B:771:SER:N	2.72	0.63
1:A:536:THR:HG22	1:A:537:GLU:H	1.61	0.63
1:A:311:ARG:NH2	1:A:597:PRO:HB2	2.13	0.63
2:B:533:SER:O	2:B:537:ILE:HG13	1.97	0.63
1:A:356:GLY:O	1:A:360:MET:HG3	1.98	0.63
1:A:392:LYS:HD3	1:A:396:GLY:C	2.19	0.62
1:A:565:PRO:HD3	1:A:761:VAL:HG21	1.81	0.62
2:B:386:CYS:SG	2:B:388:PHE:HD1	2.22	0.62
2:B:314:ARG:NH1	2:B:782:GLU:OE2	2.33	0.62
2:B:1000:VAL:HG13	2:B:1001:PHE:N	2.14	0.62
2:B:446:MET:HE1	2:B:578:LEU:HD13	1.81	0.62
2:B:1032:LEU:HG	2:B:1033:ASN:N	2.15	0.62
2:B:946:ASN:CG	2:B:946:ASN:O	2.37	0.62
1:A:311:ARG:NH1	1:A:598:ASP:OD1	2.27	0.61
2:B:699:GLY:HA3	2:B:738:LEU:HD23	1.82	0.61
2:B:590:ALA:CB	2:B:591:PRO:CD	2.74	0.61
1:A:238:MET:CE	1:A:238:MET:HA	2.29	0.61
2:B:992:LYS:HB2	2:B:996:GLN:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:ARG:HH12	2:B:742:SER:C	2.04	0.61
1:A:749:LEU:HD12	1:A:749:LEU:C	2.18	0.61
1:A:696:LEU:HD23	1:A:703:PRO:HG2	1.83	0.60
1:A:388:ARG:NH1	1:A:699:ARG:O	2.34	0.60
2:B:599:ASP:HB3	2:B:601:LYS:HG3	1.83	0.60
2:B:963:VAL:HG12	2:B:964:GLY:H	1.67	0.60
1:A:392:LYS:HD3	1:A:396:GLY:O	2.01	0.60
1:A:673:GLN:CD	1:A:673:GLN:H	2.03	0.60
2:B:861:GLU:CG	2:B:861:GLU:O	2.42	0.60
1:A:66:CYS:SG	3:A:801:ZN:ZN	1.85	0.60
2:B:770:CYS:SG	2:B:771:SER:N	2.73	0.60
2:B:709:ILE:HG22	2:B:719:MET:HG2	1.84	0.60
1:A:389:VAL:HG12	1:A:389:VAL:O	2.01	0.59
2:B:523:LEU:O	2:B:524:ASP:HB2	2.02	0.59
2:B:518:VAL:CG1	2:B:519:PHE:N	2.65	0.59
1:A:290:ILE:CD1	1:A:360:MET:CE	2.80	0.59
2:B:307:ASN:HB3	2:B:766:LEU:HD12	1.83	0.59
2:B:633:VAL:H	2:B:655:THR:CG2	2.14	0.59
2:B:2:MET:HG2	2:B:1017:TYR:OH	2.02	0.59
1:A:183:ILE:CD1	2:B:547:MET:CE	2.81	0.58
1:A:543:LEU:HD21	1:A:585:ARG:HB2	1.85	0.58
2:B:317:THR:HG22	2:B:319:CYS:H	1.67	0.58
2:B:493:LYS:HA	2:B:557:VAL:HG22	1.85	0.58
1:A:290:ILE:CD1	1:A:360:MET:HE1	2.33	0.58
2:B:947:VAL:HG12	2:B:948:PRO:HD2	1.84	0.58
2:B:489:ILE:HD11	2:B:526:PHE:CZ	2.36	0.58
2:B:601:LYS:CA	2:B:605:THR:HG21	2.33	0.58
2:B:633:VAL:HG12	2:B:655:THR:HG21	1.86	0.58
1:A:652:THR:CG2	1:A:655:GLN:O	2.51	0.58
2:B:301:MET:HG3	2:B:347:ASN:HD21	1.68	0.58
2:B:591:PRO:CG	2:B:591:PRO:O	2.51	0.58
2:B:944:ILE:CG2	2:B:945:PHE:CE1	2.87	0.58
1:A:681:PHE:O	1:A:685:LEU:HG	2.04	0.58
2:B:470:LEU:O	2:B:473:ILE:HG13	2.03	0.58
1:A:564:ASP:HB3	1:A:567:SER:CB	2.32	0.57
2:B:492:ASN:O	2:B:493:LYS:CB	2.49	0.57
2:B:996:GLN:HB3	2:B:997:PRO:CD	2.28	0.57
2:B:992:LYS:HB3	2:B:996:GLN:HG3	1.87	0.57
2:B:289:ARG:CZ	2:B:742:SER:O	2.52	0.57
2:B:664:ASN:N	2:B:664:ASN:HD22	2.03	0.57
1:A:35:VAL:HG21	1:A:552:ARG:CB	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:442:ALA:HA	2:B:484:ILE:HG23	1.86	0.57
2:B:643:VAL:O	2:B:643:VAL:HG12	2.02	0.57
2:B:289:ARG:NH1	2:B:742:SER:O	2.38	0.57
1:A:673:GLN:HB3	1:A:685:LEU:CD1	2.34	0.57
2:B:609:LYS:O	2:B:613:GLN:HG3	2.04	0.57
1:A:102:SER:HB3	1:A:105:ASN:CB	2.35	0.56
2:B:363:ARG:NE	2:B:370:TYR:CE1	2.72	0.56
1:A:78:TYR:OH	1:A:106:GLN:OE1	2.21	0.56
1:A:311:ARG:NH1	1:A:358:LEU:HB3	2.19	0.56
2:B:431:TYR:HB3	2:B:751:LEU:HD11	1.87	0.56
1:A:148:LYS:O	1:A:152:GLN:HG3	2.05	0.56
1:A:236:ILE:HG22	1:A:236:ILE:O	2.04	0.56
1:A:84:ALA:HB2	1:A:91:ARG:HD3	1.88	0.56
2:B:948:PRO:HG2	2:B:952:HIS:CD2	2.40	0.56
1:A:183:ILE:HD12	2:B:547:MET:HE1	1.88	0.56
1:A:102:SER:CB	1:A:105:ASN:H	2.18	0.56
1:A:155:LEU:HD21	1:A:240:LEU:HD23	1.88	0.56
1:A:179:GLY:HA2	1:A:236:ILE:CD1	2.34	0.56
2:B:902:MET:O	2:B:903:LEU:HG	2.05	0.56
1:A:312:SER:OG	1:A:315:ASP:CG	2.43	0.56
2:B:523:LEU:HD23	2:B:523:LEU:C	2.26	0.56
2:B:470:LEU:HD12	2:B:530:TYR:HE1	1.70	0.56
1:A:568:PHE:CD1	1:A:569:ARG:N	2.75	0.55
1:A:179:GLY:HA3	1:A:236:ILE:HD11	1.88	0.55
1:A:311:ARG:CG	1:A:311:ARG:HH21	2.12	0.55
2:B:377:PHE:HB3	2:B:403:LEU:HD21	1.88	0.55
2:B:465:GLU:O	2:B:468:THR:HB	2.06	0.55
1:A:310:ILE:HG22	1:A:311:ARG:H	1.69	0.55
1:A:363:CYS:HB2	1:A:364:PRO:CD	2.37	0.55
1:A:671:GLY:C	1:A:673:GLN:OE1	2.45	0.55
1:A:755:HIS:O	1:A:759:LEU:HG	2.07	0.55
2:B:289:ARG:NH1	2:B:742:SER:C	2.60	0.55
2:B:999:MET:SD	2:B:1002:ARG:CZ	2.95	0.55
1:A:652:THR:HG21	1:A:655:GLN:HB3	1.89	0.55
2:B:822:ARG:O	2:B:826:ALA:CB	2.52	0.55
1:A:369:GLY:O	1:A:609:ARG:NH2	2.39	0.54
1:A:413:GLU:N	1:A:413:GLU:OE1	2.29	0.54
1:A:313:TRP:CD1	1:A:592:VAL:O	2.60	0.54
1:A:121:VAL:CG2	1:A:494:ILE:HG13	2.37	0.54
1:A:121:VAL:HG12	1:A:122:LEU:N	2.23	0.54
1:A:652:THR:HG22	1:A:655:GLN:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:CYS:O	1:A:89:TYR:HA	2.08	0.54
1:A:95:PRO:HG2	1:A:98:TYR:CD1	2.43	0.54
1:A:153:MET:HG3	1:A:154:SER:N	2.22	0.54
1:A:183:ILE:HD12	2:B:547:MET:CE	2.38	0.54
1:A:556:LYS:HG2	1:A:557:PHE:CE2	2.43	0.54
1:A:519:GLN:OE1	1:A:576:LEU:HB2	2.08	0.54
2:B:941:ILE:HG23	2:B:953:ILE:HD11	1.90	0.54
1:A:311:ARG:NH2	1:A:354:GLN:OE1	2.39	0.54
1:A:404:GLY:HA2	1:A:484:GLN:O	2.08	0.54
1:A:107:PRO:CD	1:A:110:LEU:HD12	2.37	0.54
2:B:686:ILE:HG22	2:B:687:GLY:N	2.23	0.54
2:B:871:ARG:O	2:B:875:MET:CE	2.56	0.54
2:B:996:GLN:CB	2:B:997:PRO:HD2	2.30	0.54
1:A:54:ILE:HG13	1:A:117:ILE:HD11	1.88	0.54
1:A:238:MET:CE	1:A:238:MET:CA	2.85	0.54
1:A:606:HIS:O	1:A:610:GLN:HG2	2.08	0.54
2:B:644:ASP:OD1	2:B:647:SER:HB2	2.07	0.54
2:B:686:ILE:CG2	2:B:687:GLY:N	2.71	0.54
1:A:524:ILE:HG13	1:A:612:LEU:HD12	1.88	0.53
2:B:415:LYS:HB2	2:B:418:LEU:HD12	1.90	0.53
2:B:633:VAL:CG1	2:B:655:THR:HG21	2.39	0.53
2:B:307:ASN:OD1	2:B:767:GLY:N	2.35	0.53
1:A:363:CYS:HB2	1:A:364:PRO:HD3	1.89	0.53
1:A:388:ARG:NH2	1:A:702:MET:HG3	2.24	0.53
2:B:963:VAL:HG12	2:B:964:GLY:N	2.24	0.53
1:A:311:ARG:NH1	1:A:356:GLY:HA2	2.23	0.53
1:A:573:THR:HG22	1:A:574:PHE:CD1	2.43	0.53
2:B:384:TYR:CZ	2:B:393:ASN:HB2	2.44	0.53
2:B:653:GLN:HB2	2:B:872:GLN:NE2	2.23	0.53
2:B:470:LEU:HD13	2:B:530:TYR:CD1	2.44	0.53
2:B:693:ARG:NH1	2:B:695:ARG:NE	2.56	0.53
1:A:388:ARG:O	1:A:391:THR:N	2.38	0.53
2:B:464:GLU:CD	2:B:467:LYS:NZ	2.62	0.53
1:A:313:TRP:O	1:A:316:ILE:HG22	2.08	0.53
2:B:377:PHE:CD2	2:B:409:ARG:HD2	2.44	0.53
2:B:401:GLN:HB2	2:B:409:ARG:NH2	2.23	0.53
2:B:652:PRO:HA	2:B:655:THR:HG22	1.91	0.53
1:A:528:ARG:HG2	1:A:608:MET:HE2	1.91	0.52
2:B:944:ILE:HG21	2:B:945:PHE:CE1	2.44	0.52
1:A:183:ILE:HD13	2:B:547:MET:SD	2.49	0.52
1:A:524:ILE:HG13	1:A:612:LEU:CD1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:612:LEU:HA	1:A:615:SER:OG	2.09	0.52
1:A:652:THR:CG2	1:A:655:GLN:H	2.12	0.52
1:A:102:SER:HB3	1:A:105:ASN:N	2.25	0.52
1:A:653:PHE:HA	1:A:699:ARG:NH1	2.24	0.52
2:B:899:LYS:O	2:B:900:SER:CB	2.57	0.52
1:A:33:ARG:O	1:A:556:LYS:HD3	2.09	0.52
2:B:500:VAL:CG1	2:B:537:ILE:HG12	2.38	0.52
2:B:605:THR:O	2:B:606:ASP:HB3	2.10	0.52
2:B:962:GLU:HB3	2:B:963:VAL:CG2	2.40	0.52
2:B:322:CYS:SG	2:B:771:SER:O	2.67	0.52
1:A:239:ASN:HD22	1:A:239:ASN:N	2.06	0.52
1:A:60:LEU:HB3	1:A:67:ARG:HH11	1.73	0.52
2:B:301:MET:HG3	2:B:347:ASN:ND2	2.24	0.52
1:A:543:LEU:CD2	1:A:585:ARG:HB2	2.41	0.51
1:A:311:ARG:CG	1:A:311:ARG:NH2	2.73	0.51
1:A:358:LEU:HD22	1:A:597:PRO:HB3	1.91	0.51
1:A:384:GLN:O	1:A:388:ARG:HG2	2.09	0.51
1:A:656:ILE:HD11	1:A:695:ILE:HG21	1.90	0.51
2:B:699:GLY:O	2:B:735:ASP:O	2.28	0.51
1:A:476:ARG:HG2	1:A:502:ASN:OD1	2.10	0.51
1:A:77:ASP:CG	1:A:79:ARG:O	2.49	0.51
2:B:944:ILE:CG2	2:B:945:PHE:CD1	2.92	0.51
1:A:166:LEU:HD23	1:A:243:LEU:CD2	2.40	0.51
1:A:564:ASP:O	1:A:567:SER:CA	2.59	0.51
1:A:591:GLN:NE2	1:A:591:GLN:HA	2.25	0.51
2:B:443:PHE:CG	2:B:579:PHE:HE2	2.28	0.51
2:B:834:LEU:HD11	2:B:1025:HIS:HB2	1.93	0.51
2:B:942:GLN:CG	2:B:948:PRO:HA	2.40	0.51
1:A:533:ARG:HD3	1:A:538:GLU:OE2	2.11	0.51
2:B:979:GLN:HE22	2:B:985:SER:HA	1.74	0.51
2:B:627:VAL:HG21	2:B:710:LEU:HD23	1.93	0.51
1:A:743:LEU:HD12	1:A:759:LEU:HD12	1.93	0.51
2:B:962:GLU:HB3	2:B:963:VAL:HG22	1.93	0.51
1:A:297:GLY:CA	1:A:300:MET:HB2	2.40	0.51
2:B:469:MET:HE3	2:B:678:LEU:C	2.30	0.51
1:A:179:GLY:CA	1:A:236:ILE:CD1	2.87	0.51
2:B:453:ASN:ND2	2:B:583:SER:HB3	2.25	0.51
2:B:704:ASP:HB2	2:B:731:GLU:HB3	1.93	0.51
2:B:523:LEU:HD23	2:B:524:ASP:N	2.26	0.51
2:B:590:ALA:HB1	2:B:591:PRO:HD3	1.91	0.51
1:A:51:LEU:CD1	1:A:114:PHE:HE1	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:607:LYS:HG2	2:B:610:ILE:HG13	1.93	0.50
1:A:313:TRP:HA	1:A:316:ILE:HG22	1.92	0.50
1:A:51:LEU:HD12	1:A:52:PRO:HD3	1.92	0.50
1:A:584:LEU:O	1:A:587:SER:OG	2.29	0.50
2:B:818:LEU:HD22	2:B:836:LEU:HD22	1.92	0.50
2:B:958:THR:O	2:B:958:THR:HG22	2.11	0.50
2:B:302:ILE:HD13	2:B:310:PRO:HD2	1.94	0.50
2:B:470:LEU:HD13	2:B:530:TYR:CE1	2.45	0.50
2:B:944:ILE:HG22	2:B:945:PHE:CE1	2.44	0.50
1:A:35:VAL:CG2	1:A:552:ARG:HB3	2.37	0.50
2:B:366:ARG:HH21	2:B:391:CYS:CB	2.21	0.50
2:B:949:SER:N	2:B:952:HIS:HD2	2.07	0.50
2:B:602:LEU:HA	2:B:608:GLU:HB2	1.94	0.50
2:B:947:VAL:HG11	2:B:952:HIS:HB3	1.93	0.50
1:A:302:VAL:CG2	1:A:303:GLY:N	2.74	0.49
2:B:638:PHE:HZ	2:B:674:PHE:CE1	2.29	0.49
1:A:190:ARG:NH1	2:B:517:GLU:HG2	2.27	0.49
1:A:238:MET:HE2	1:A:238:MET:CA	2.41	0.49
1:A:311:ARG:HH11	1:A:356:GLY:HA2	1.76	0.49
2:B:973:MET:O	2:B:977:ILE:N	2.46	0.49
1:A:18:ARG:NH2	1:A:518:ASP:OD1	2.42	0.49
1:A:51:LEU:HD13	1:A:114:PHE:CE1	2.47	0.49
2:B:554:ASN:N	2:B:554:ASN:ND2	2.60	0.49
1:A:426:LEU:HD21	1:A:447:LYS:HB2	1.93	0.49
1:A:77:ASP:OD1	1:A:79:ARG:O	2.29	0.49
2:B:365:ASN:N	2:B:393:ASN:OD1	2.44	0.49
2:B:363:ARG:CZ	2:B:370:TYR:CE1	2.83	0.49
2:B:322:CYS:SG	2:B:771:SER:C	2.90	0.49
2:B:942:GLN:HE21	2:B:948:PRO:HA	1.77	0.49
2:B:889:GLN:O	2:B:922:LEU:HA	2.12	0.49
1:A:239:ASN:N	1:A:239:ASN:ND2	2.60	0.49
1:A:448:ILE:HD11	1:A:457:LEU:HD11	1.94	0.49
2:B:726:LYS:CD	2:B:876:THR:HG21	2.43	0.49
1:A:700:PHE:CD1	1:A:700:PHE:C	2.85	0.49
2:B:945:PHE:O	2:B:946:ASN:HB3	2.11	0.49
1:A:51:LEU:HD12	1:A:114:PHE:CE1	2.48	0.49
1:A:389:VAL:O	1:A:389:VAL:CG1	2.61	0.49
1:A:78:TYR:HD1	1:A:101:ILE:HG12	1.77	0.49
2:B:621:SER:O	2:B:624:LYS:HB2	2.12	0.49
2:B:928:MET:O	2:B:988:LEU:HD12	2.13	0.49
2:B:614:PRO:HA	2:B:647:SER:OG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ARG:C	1:A:390:PHE:N	2.64	0.48
2:B:528:VAL:HG12	2:B:529:ASN:N	2.27	0.48
1:A:123:ARG:HG3	1:A:125:PRO:CD	2.40	0.48
1:A:388:ARG:HH22	1:A:702:MET:HG3	1.78	0.48
2:B:389:CYS:O	2:B:390:ASN:HB2	2.13	0.48
1:A:388:ARG:C	1:A:390:PHE:H	2.17	0.48
1:A:573:THR:HG22	1:A:574:PHE:CE1	2.49	0.48
2:B:289:ARG:HD2	2:B:769:ASN:OD1	2.13	0.48
1:A:290:ILE:CD1	1:A:360:MET:HE3	2.43	0.48
1:A:564:ASP:N	1:A:565:PRO:CD	2.76	0.48
1:A:692:ALA:O	1:A:696:LEU:HG	2.13	0.48
2:B:600:LYS:HG3	2:B:600:LYS:O	2.14	0.48
1:A:500:ALA:O	1:A:501:ARG:NH1	2.44	0.48
2:B:612:PHE:CD1	2:B:871:ARG:HD3	2.49	0.48
1:A:131:PHE:CD2	1:A:158:LEU:HD22	2.48	0.48
2:B:1009:LYS:HG2	2:B:1016:SER:HB3	1.96	0.48
2:B:654:LEU:HD13	2:B:710:LEU:HD13	1.95	0.48
2:B:820:CYS:O	2:B:824:ASN:HB2	2.14	0.48
2:B:965:ASN:N	2:B:966:PRO:CD	2.77	0.48
1:A:77:ASP:O	1:A:79:ARG:O	2.32	0.48
1:A:107:PRO:CG	1:A:110:LEU:HD12	2.44	0.47
1:A:183:ILE:HD13	2:B:547:MET:CE	2.44	0.47
1:A:262:ARG:CZ	1:A:292:GLY:HA3	2.44	0.47
1:A:452:SER:C	1:A:454:THR:H	2.16	0.47
2:B:523:LEU:HD23	2:B:524:ASP:OD1	2.14	0.47
2:B:427:ALA:HB3	2:B:759:ARG:HB3	1.96	0.47
1:A:102:SER:HB3	1:A:105:ASN:CA	2.44	0.47
1:A:66:CYS:SG	1:A:88:CYS:SG	3.11	0.47
1:A:589:PHE:O	1:A:590:LEU:HD23	2.15	0.47
2:B:375:MET:CE	2:B:386:CYS:SG	3.02	0.47
2:B:289:ARG:NH2	2:B:742:SER:O	2.47	0.47
2:B:537:ILE:HG22	2:B:541:LEU:HD12	1.96	0.47
1:A:290:ILE:HD13	1:A:360:MET:HE3	1.95	0.47
2:B:949:SER:H	2:B:952:HIS:HD2	1.61	0.47
2:B:967:TYR:O	2:B:970:GLN:N	2.44	0.47
1:A:154:SER:O	1:A:158:LEU:HG	2.14	0.47
1:A:556:LYS:HG2	1:A:557:PHE:CZ	2.50	0.47
2:B:1025:HIS:HA	2:B:1028:ILE:HD12	1.96	0.47
2:B:966:PRO:HG2	2:B:967:TYR:H	1.80	0.47
2:B:999:MET:SD	2:B:1002:ARG:NH1	2.88	0.47
2:B:522:LEU:HD11	2:B:526:PHE:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:SER:HB3	1:A:105:ASN:HB2	1.96	0.47
2:B:642:TYR:OH	2:B:644:ASP:OD2	2.31	0.47
1:A:169:PHE:C	1:A:169:PHE:CD1	2.88	0.47
2:B:462:ILE:O	2:B:466:LEU:HB2	2.15	0.47
2:B:547:MET:HE3	2:B:547:MET:HB2	1.69	0.47
2:B:606:ASP:HA	2:B:802:PRO:HG3	1.97	0.47
1:A:560:TYR:CD1	1:A:560:TYR:N	2.82	0.46
2:B:280:GLY:O	2:B:282:GLN:HG3	2.15	0.46
2:B:469:MET:CE	2:B:678:LEU:HG	2.45	0.46
2:B:822:ARG:HD2	2:B:822:ARG:HA	1.73	0.46
1:A:44:PRO:O	1:A:45:LEU:HD23	2.15	0.46
2:B:907:VAL:HG12	2:B:908:ARG:N	2.31	0.46
1:A:363:CYS:CB	1:A:364:PRO:CD	2.93	0.46
1:A:591:GLN:HE21	1:A:591:GLN:HA	1.80	0.46
2:B:374:PHE:CD2	2:B:745:LEU:HD22	2.50	0.46
2:B:478:GLN:HE22	2:B:758:GLN:HE22	1.63	0.46
2:B:965:ASN:H	2:B:966:PRO:CD	2.29	0.46
1:A:113:GLN:H	1:A:113:GLN:HG2	1.52	0.46
1:A:166:LEU:HD23	1:A:243:LEU:HD21	1.97	0.46
1:A:276:GLU:HG3	1:A:341:THR:HG21	1.97	0.46
1:A:644:ALA:O	1:A:663:THR:HB	2.15	0.46
2:B:614:PRO:HG3	2:B:650:LEU:HD22	1.98	0.46
2:B:723:ASP:OD1	2:B:725:ASP:HB2	2.16	0.46
2:B:959:LEU:O	2:B:960:LEU:C	2.54	0.46
1:A:238:MET:O	1:A:242:ASP:OD2	2.34	0.46
1:A:622:ILE:HG21	1:A:624:TYR:CZ	2.51	0.46
2:B:625:ASP:O	2:B:628:ALA:HB3	2.16	0.46
2:B:637:LEU:HG	2:B:639:PRO:HD3	1.97	0.46
2:B:726:LYS:HD3	2:B:876:THR:HG21	1.96	0.46
1:A:452:SER:O	1:A:454:THR:N	2.49	0.46
1:A:705:TYR:HE1	1:A:707:ASP:HB2	1.81	0.46
1:A:81:LYS:HE2	1:A:99:ALA:HA	1.98	0.46
2:B:354:VAL:HG22	2:B:416:PRO:HG2	1.98	0.46
2:B:916:GLU:O	2:B:935:SER:HB2	2.16	0.46
1:A:554:CYS:O	1:A:558:GLY:N	2.48	0.46
1:A:155:LEU:HD12	1:A:158:LEU:HD12	1.98	0.46
2:B:284:TYR:CZ	2:B:291:GLN:OE1	2.69	0.46
2:B:310:PRO:HA	2:B:313:ILE:O	2.16	0.46
2:B:606:ASP:OD1	2:B:802:PRO:HG3	2.16	0.46
2:B:286:THR:OG1	2:B:286:THR:O	2.33	0.45
2:B:854:CYS:SG	2:B:870:GLN:OE1	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:PRO:HD3	1:A:109:GLU:O	2.16	0.45
2:B:965:ASN:N	2:B:966:PRO:HD2	2.32	0.45
1:A:21:TRP:CZ3	1:A:517:PHE:HB2	2.51	0.45
1:A:653:PHE:O	1:A:699:ARG:NH1	2.45	0.45
1:A:657:LEU:HD23	1:A:658:ILE:N	2.31	0.45
1:A:662:GLU:HB2	1:A:710:HIS:ND1	2.32	0.45
2:B:518:VAL:HG21	2:B:560:PRO:HB3	1.98	0.45
1:A:162:ALA:O	1:A:232:PRO:HA	2.17	0.45
1:A:302:VAL:HG22	1:A:303:GLY:H	1.79	0.45
1:A:79:ARG:O	1:A:80:ALA:HB3	2.16	0.45
1:A:121:VAL:HG23	1:A:494:ILE:HG13	1.99	0.45
2:B:469:MET:HE2	2:B:679:ARG:HA	1.96	0.45
1:A:18:ARG:HH21	1:A:518:ASP:CG	2.20	0.45
1:A:392:LYS:HD3	1:A:396:GLY:CA	2.47	0.45
1:A:565:PRO:C	1:A:567:SER:N	2.69	0.45
2:B:458:LEU:O	2:B:462:ILE:HG13	2.17	0.45
2:B:893:ILE:HB	2:B:919:ILE:HG22	1.99	0.45
2:B:996:GLN:CB	2:B:997:PRO:CD	2.94	0.45
1:A:712:GLY:C	1:A:714:GLN:N	2.70	0.45
1:A:33:ARG:HD3	1:A:33:ARG:HA	1.73	0.45
1:A:652:THR:HG23	1:A:655:GLN:O	2.15	0.45
2:B:1022:CYS:O	2:B:1026:LYS:HG3	2.17	0.45
2:B:388:PHE:N	2:B:388:PHE:CD1	2.84	0.45
1:A:529:LEU:HD23	1:A:529:LEU:HA	1.88	0.45
1:A:83:TRP:CE2	1:A:92:ASN:HB2	2.52	0.45
2:B:364:CYS:SG	2:B:386:CYS:HB2	2.56	0.45
2:B:453:ASN:HD21	2:B:583:SER:HB3	1.82	0.45
2:B:601:LYS:HA	2:B:605:THR:HG21	1.98	0.45
2:B:664:ASN:N	2:B:664:ASN:ND2	2.65	0.45
2:B:726:LYS:HD2	2:B:876:THR:CG2	2.47	0.45
1:A:568:PHE:HD1	1:A:569:ARG:N	2.14	0.44
2:B:284:TYR:CE1	2:B:291:GLN:OE1	2.70	0.44
2:B:947:VAL:CG1	2:B:948:PRO:HD2	2.45	0.44
2:B:528:VAL:CG1	2:B:533:SER:OG	2.62	0.44
1:A:254:VAL:HA	1:A:255:PRO:HD2	1.66	0.44
1:A:35:VAL:CG1	1:A:549:GLN:HE21	2.29	0.44
1:A:540:PRO:C	1:A:542:VAL:H	2.21	0.44
1:A:584:LEU:HD13	1:A:619:ILE:HD11	2.00	0.44
2:B:1032:LEU:O	2:B:1033:ASN:HB2	2.17	0.44
2:B:282:GLN:O	2:B:300:CYS:HB2	2.18	0.44
2:B:488:PHE:C	2:B:489:ILE:HG13	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:602:LEU:N	2:B:605:THR:CG2	2.79	0.44
2:B:829:SER:HB2	2:B:833:GLN:OE1	2.17	0.44
1:A:700:PHE:CD1	1:A:700:PHE:O	2.70	0.44
2:B:813:GLN:O	2:B:817:MET:HG3	2.17	0.44
1:A:530:ALA:HB2	1:A:546:LEU:HD13	1.99	0.44
2:B:403:LEU:HD13	2:B:407:GLY:HA2	2.00	0.44
2:B:453:ASN:O	2:B:459:VAL:HG23	2.18	0.44
1:A:252:TRP:HA	1:A:253:PRO:HD3	1.78	0.43
2:B:1000:VAL:CG1	2:B:1001:PHE:N	2.79	0.43
2:B:523:LEU:CD2	2:B:524:ASP:CG	2.86	0.43
2:B:589:GLU:HG2	2:B:593:LYS:NZ	2.32	0.43
1:A:311:ARG:NE	1:A:359:GLU:OE2	2.49	0.43
1:A:47:GLU:HG2	1:A:453:PRO:HB3	2.00	0.43
1:A:589:PHE:C	1:A:590:LEU:HD23	2.39	0.43
1:A:60:LEU:CB	1:A:67:ARG:NH1	2.77	0.43
2:B:520:VAL:HG12	2:B:522:LEU:H	1.83	0.43
2:B:523:LEU:HD23	2:B:524:ASP:CG	2.38	0.43
2:B:1024:VAL:CG1	2:B:1028:ILE:HD11	2.40	0.43
2:B:570:LYS:HE2	2:B:629:HIS:NE2	2.33	0.43
1:A:312:SER:H	1:A:315:ASP:HB2	1.82	0.43
1:A:314:HIS:HB3	1:A:318:LYS:NZ	2.33	0.43
1:A:518:ASP:HB3	1:A:521:ALA:HB3	1.99	0.43
1:A:102:SER:CB	1:A:105:ASN:HB2	2.48	0.43
1:A:564:ASP:CG	1:A:567:SER:HB3	2.38	0.43
2:B:902:MET:O	2:B:903:LEU:CG	2.66	0.43
2:B:469:MET:O	2:B:470:LEU:C	2.56	0.43
2:B:543:GLN:HB3	2:B:547:MET:CE	2.49	0.43
1:A:370:TYR:CE2	1:A:389:VAL:HG13	2.46	0.43
1:A:81:LYS:HZ1	1:A:99:ALA:HB1	1.84	0.43
2:B:469:MET:SD	2:B:678:LEU:HG	2.59	0.43
2:B:933:GLY:O	2:B:936:SER:OG	2.30	0.43
1:A:297:GLY:HA3	1:A:300:MET:HB2	2.01	0.42
1:A:647:ILE:HG21	1:A:688:PRO:HG3	2.00	0.42
2:B:731:GLU:HB2	2:B:789:PHE:HE1	1.83	0.42
1:A:51:LEU:CD1	1:A:52:PRO:HD2	2.46	0.42
1:A:240:LEU:O	1:A:243:LEU:HB3	2.19	0.42
1:A:3:THR:HG22	1:A:5:LEU:H	1.84	0.42
2:B:441:PRO:HA	2:B:575:PRO:O	2.18	0.42
1:A:111:LEU:HA	1:A:112:PRO:HD3	1.92	0.42
1:A:672:TYR:N	1:A:673:GLN:OE1	2.53	0.42
2:B:470:LEU:O	2:B:471:GLU:C	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:496:HIS:CE1	2:B:548:PHE:CE2	3.08	0.42
2:B:911:GLU:HA	2:B:914:LEU:HD12	2.00	0.42
1:A:169:PHE:CD2	1:A:267:ALA:CB	3.03	0.42
1:A:194:ASP:OD1	1:A:195:LEU:N	2.53	0.42
1:A:416:ILE:O	1:A:434:SER:HB3	2.20	0.42
1:A:751:VAL:O	1:A:752:PHE:C	2.57	0.42
2:B:1015:SER:HB2	2:B:1019:ASP:HB3	2.01	0.42
2:B:375:MET:SD	2:B:386:CYS:HA	2.59	0.42
1:A:637:LEU:O	1:A:722:VAL:HG13	2.19	0.42
2:B:821:TYR:CD1	2:B:837:PRO:HD3	2.54	0.42
1:A:363:CYS:CB	1:A:364:PRO:HD3	2.49	0.42
2:B:410:LEU:O	2:B:411:ASP:CB	2.68	0.42
2:B:515:VAL:HG12	2:B:516:GLY:N	2.35	0.42
1:A:23:VAL:HG12	1:A:513:ILE:HG12	2.01	0.42
1:A:60:LEU:HD23	1:A:67:ARG:HG3	2.00	0.42
2:B:845:VAL:HG13	2:B:1017:TYR:CD1	2.55	0.42
2:B:723:ASP:OD2	2:B:726:LYS:HE2	2.20	0.42
2:B:907:VAL:HG11	2:B:913:ARG:HB3	2.01	0.42
1:A:25:PRO:HG3	1:A:34:MET:SD	2.60	0.42
2:B:585:LEU:HA	2:B:586:PRO:HD2	1.80	0.41
2:B:600:LYS:HD2	2:B:602:LEU:HD23	2.02	0.41
2:B:374:PHE:CE2	2:B:745:LEU:HD22	2.56	0.41
2:B:810:LEU:HD23	2:B:810:LEU:HA	1.86	0.41
2:B:960:LEU:HA	2:B:961:PRO:HD3	1.62	0.41
2:B:949:SER:O	2:B:950:PHE:C	2.57	0.41
2:B:569:LEU:HD22	2:B:576:GLY:HA3	2.01	0.41
2:B:798:VAL:HG13	2:B:803:LEU:HD21	2.03	0.41
2:B:942:GLN:HG2	2:B:948:PRO:HA	2.01	0.41
2:B:960:LEU:HD12	2:B:960:LEU:H	1.85	0.41
1:A:666:GLN:HA	1:A:669:LYS:HB2	2.02	0.41
2:B:617:ASN:HD22	2:B:617:ASN:C	2.15	0.41
2:B:693:ARG:HD2	2:B:716:ASP:OD1	2.19	0.41
2:B:726:LYS:HA	2:B:876:THR:HG22	2.03	0.41
2:B:947:VAL:CG1	2:B:952:HIS:CB	2.98	0.41
2:B:966:PRO:HG2	2:B:967:TYR:N	2.35	0.41
1:A:290:ILE:HD13	1:A:360:MET:CE	2.48	0.41
1:A:392:LYS:HD3	1:A:396:GLY:HA2	2.02	0.41
1:A:568:PHE:C	1:A:568:PHE:CD1	2.93	0.41
1:A:656:ILE:HA	1:A:656:ILE:HD13	1.94	0.41
1:A:679:GLU:OE1	1:A:682:ARG:NH1	2.53	0.41
1:A:673:GLN:CB	1:A:685:LEU:HD12	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:LEU:HD11	1:A:500:ALA:HB2	2.00	0.41
2:B:523:LEU:CD2	2:B:523:LEU:C	2.89	0.41
2:B:605:THR:O	2:B:606:ASP:CB	2.68	0.41
2:B:947:VAL:HG11	2:B:952:HIS:CB	2.50	0.41
1:A:438:ILE:HG21	1:A:529:LEU:HD21	2.02	0.41
2:B:469:MET:HE1	2:B:678:LEU:HG	2.03	0.41
2:B:585:LEU:HD21	2:B:594:LEU:HB2	2.03	0.41
2:B:607:LYS:HE2	2:B:610:ILE:CD1	2.48	0.41
1:A:178:LEU:C	1:A:180:CYS:H	2.23	0.41
1:A:712:GLY:C	1:A:714:GLN:H	2.23	0.41
1:A:612:LEU:O	1:A:615:SER:OG	2.28	0.41
1:A:657:LEU:C	1:A:657:LEU:CD2	2.85	0.41
2:B:441:PRO:HG2	2:B:484:ILE:HG12	2.02	0.41
1:A:17:VAL:HG13	1:A:19:PHE:CD1	2.56	0.41
1:A:658:ILE:HD12	1:A:705:TYR:OH	2.20	0.41
2:B:787:ILE:HG13	2:B:846:TYR:HB3	2.03	0.41
1:A:123:ARG:CG	1:A:125:PRO:HD2	2.45	0.40
1:A:155:LEU:CD2	1:A:240:LEU:HD23	2.50	0.40
1:A:259:ARG:HG3	1:A:306:LEU:HD23	2.02	0.40
1:A:388:ARG:O	1:A:389:VAL:C	2.56	0.40
2:B:492:ASN:C	2:B:492:ASN:OD1	2.53	0.40
2:B:443:PHE:HB3	2:B:579:PHE:CE2	2.56	0.40
2:B:577:LYS:HA	2:B:632:SER:O	2.21	0.40
2:B:693:ARG:HH12	2:B:695:ARG:NE	2.19	0.40
2:B:942:GLN:O	2:B:946:ASN:CA	2.67	0.40
1:A:427:ASN:HA	1:A:443:THR:HB	2.03	0.40
2:B:645:VAL:O	2:B:645:VAL:HG12	2.20	0.40
1:A:576:LEU:HD23	1:A:576:LEU:HA	1.81	0.40
2:B:845:VAL:HG22	2:B:1017:TYR:CE1	2.55	0.40
2:B:334:LEU:HD22	2:B:334:LEU:H	1.86	0.40
2:B:651:VAL:O	2:B:655:THR:HB	2.21	0.40
2:B:787:ILE:HA	2:B:787:ILE:HD13	1.80	0.40
1:A:407:GLU:OE2	1:A:409:LYS:HE3	2.21	0.40
1:A:594:ASN:O	1:A:595:ASN:ND2	2.50	0.40
2:B:1032:LEU:O	2:B:1033:ASN:CB	2.69	0.40
2:B:475:LYS:O	2:B:475:LYS:HG3	2.21	0.40
1:A:745:ASP:O	1:A:746:ASP:C	2.58	0.40
1:A:190:ARG:NH1	2:B:517:GLU:O	2.54	0.40
2:B:661:LYS:HZ1	2:B:663:ASN:HD21	1.69	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%)	666 (94%)	39 (6%)	3 (0%)	39	79
2	B	763/770 (99%)	718 (94%)	39 (5%)	6 (1%)	24	67
All	All	1471/1535 (96%)	1384 (94%)	78 (5%)	9 (1%)	30	72

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	304	ASP
2	B	411	ASP
2	B	968	SER
2	B	998	GLU
1	A	389	VAL
1	A	52	PRO
2	B	965	ASN
2	B	996	GLN
1	A	540	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	624/666 (94%)	601 (96%)	23 (4%)	41	77
2	B	672/682 (98%)	645 (96%)	27 (4%)	38	75
All	All	1296/1348 (96%)	1246 (96%)	50 (4%)	39	76



All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	VAL
1	A	105	ASN
1	A	122	LEU
1	A	196	SER
1	A	201	GLN
1	A	226	SER
1	A	268	LEU
1	A	301	VAL
1	A	310	ILE
1	A	417	SER
1	A	492	ARG
1	A	567	SER
1	A	570	PHE
1	A	573	THR
1	A	616	LEU
1	A	638	ASP
1	A	639	SER
1	A	641	SER
1	A	652	THR
1	A	742	ILE
1	A	744	THR
1	A	747	VAL
1	A	749	LEU
2	B	278	SER
2	B	296	VAL
2	B	334	LEU
2	B	338	ILE
2	B	346	SER
2	B	359	SER
2	B	468	THR
2	B	554	ASN
2	B	602	LEU
2	B	617	ASN
2	B	655	THR
2	B	664	ASN
2	B	741	ASP
2	B	747	GLN
2	B	777	LEU
2	B	825	CYS
2	B	845	VAL
2	B	857	LEU
2	B	858	SER

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Mol	Chain	Res	Type
2	B	875	MET
2	B	932	LEU
2	B	963	VAL
2	B	979	GLN
2	B	982	ARG
2	B	1021	LEU
2	B	1030	GLN
2	B	1031	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	330	HIS
1	A	387	GLN
1	A	397	GLN
1	A	427	ASN
1	A	591	GLN
1	A	595	ASN
1	A	655	GLN
2	B	303	GLN
2	B	305	GLN
2	B	331	GLN
2	B	385	GLN
2	B	412	HIS
2	B	478	GLN
2	B	554	ASN
2	B	617	ASN
2	B	663	ASN
2	B	664	ASN
2	B	668	HIS
2	B	816	HIS
2	B	946	ASN
2	B	952	HIS
2	B	969	GLN
2	B	979	GLN

### 5.3.3 RNA ⓘ

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 carbohydrates 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 [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	716/765 (93%)	0.01	15 (2%) 67 61	26, 71, 129, 225	0
2	B	767/770 (99%)	0.10	34 (4%) 38 34	31, 74, 160, 275	0
All	All	1483/1535 (96%)	0.06	49 (3%) 50 45	26, 72, 149, 275	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	832	SER	8.8
2	B	1	ALA	6.9
1	A	741	PRO	6.6
1	A	742	ILE	5.9
2	B	1033	ASN	5.8
1	A	52	PRO	5.8
2	B	1014	GLY	5.4
2	B	833	GLN	5.2
2	B	1010	GLY	5.1
2	B	831	ALA	4.8
1	A	537	GLU	4.6
1	A	745	ASP	4.4
2	B	1017	TYR	4.1
2	B	902	MET	4.0
1	A	746	ASP	4.0
2	B	900	SER	3.8
2	B	1015	SER	3.8
2	B	958	THR	3.6
2	B	1021	LEU	3.6
2	B	604	ASN	3.4
1	A	744	THR	3.4
2	B	834	LEU	3.3
2	B	966	PRO	3.2
2	B	965	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	51	LEU	3.1
2	B	959	LEU	2.8
2	B	944	ILE	2.8
2	B	1020	PHE	2.7
1	A	98	TYR	2.7
1	A	743	LEU	2.6
2	B	968	SER	2.6
2	B	964	GLY	2.6
2	B	967	TYR	2.6
2	B	1016	SER	2.5
2	B	835	ILE	2.5
1	A	667	TRP	2.4
2	B	963	VAL	2.4
2	B	932	LEU	2.4
1	A	25	PRO	2.3
2	B	404	ASP	2.3
2	B	899	LYS	2.3
1	A	101	ILE	2.3
2	B	956	ASP	2.2
1	A	677	GLU	2.1
2	B	919	ILE	2.1
2	B	830	ALA	2.1
1	A	719	LEU	2.1
2	B	953	ILE	2.0
2	B	960	LEU	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	B	1101	1/1	0.83	0.12	-1.64	81,81,81,81	0
3	ZN	A	801	1/1	0.93	0.07	-2.26	70,70,70,70	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.