



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2024 – 12:08 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4.02b-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

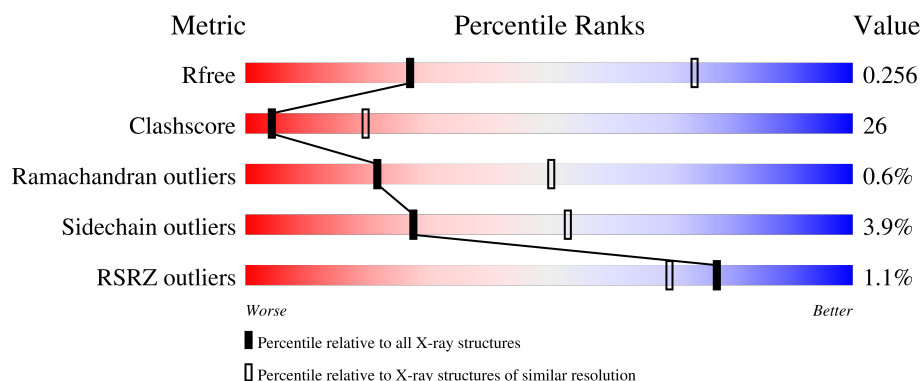
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	164625	1140 (3.46-3.34)
Clashscore	180529	1172 (3.46-3.34)
Ramachandran outliers	177936	1172 (3.46-3.34)
Sidechain outliers	177891	1172 (3.46-3.34)
RSRZ outliers	164620	1140 (3.46-3.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	765	
2	B	770	

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

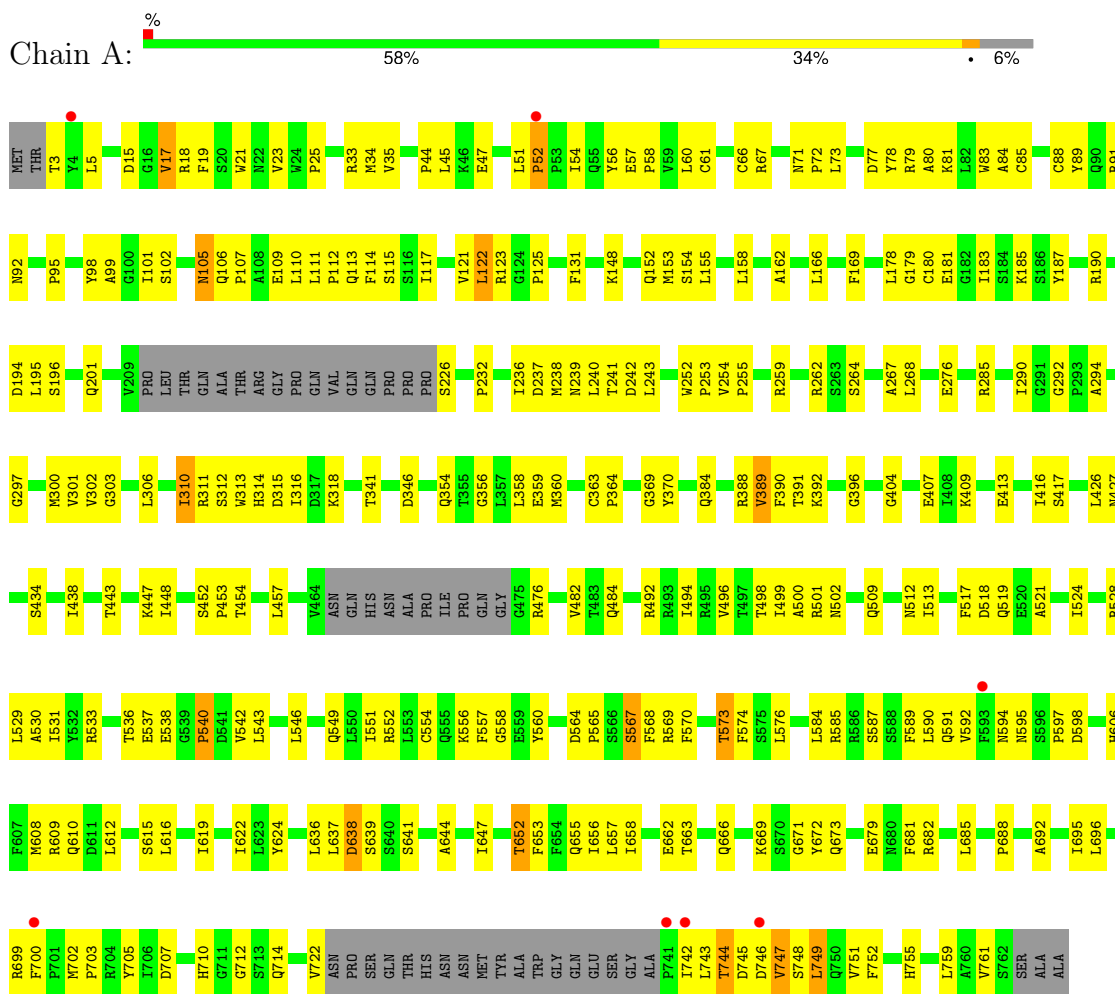
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

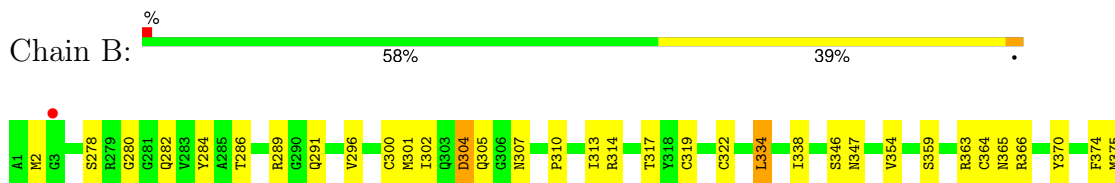
3 Residue-property plots

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: Protein transport protein Sec23A



• Molecule 2: Protein transport protein Sec24D



Q1030	T958	P860	R759	L650	G576	K472	Q376
L1031	L959	E861	R760	V651	K577	I473	F377
L1032	P961	Q870	N765	P652	L578	K474	I378
N1033	E962	R871	L766	P653	F579	K475	E379
	Y963	Q872	L768	T655	S583	Q478	R383
	G964	M875	N769	K661	S584	I484	Y384
	N965	T876	C770	T662	L585		Q385
	P966	Q889	N663	N664	T587		C386
	Y967				F488		G387
	S968				I489		F388
	Q969				T490		C389
	Q970	I893	L777	F674	E589	Y491	N390
			E782		A590	N492	C391
	M973	L896	I787	L678	G592	K493	V392
	I974	K899	F788	R679	K593	H496	N393
	N975	S900	N788	T686	L594	F497	Q401
	G976	S901	F789	G687	D599	H498	H402
	I977	M901	K792	R693	K600	N499	L403
	I978	N902	F795	V694	L602	V500	
	Q979	L903		R695	T605		I406
		V907	V798	T696	D606	G516	G407
	R982	R908		S697	K607	E517	R408
	S985			T698	E608	V518	R409
	L988	E911	P802	G699	L610	F519	L410
	N989	S912	L803		P521	V520	D411
	K992	R913	L810	T703	L611		H412
	Q993	L914	Q813	D704	F612	K415	
		S915			Q613	P416	K415
		E916			F614	E417	E417
	Q996	I919	M817	T709	Q617	S419	
	P997	F920	L818	L710	Q613		L418
	E998	L921	A819	D716	F526		L418
	N999	L922	C820		L527		
	V1000		Y821	M719	N529		A427
	F1001		R822		Y530		Y431
	R1002	M928	K823	D723	S533		P441
			N824	C724			A442
	K1009	W931	C825	D725			F443
	G1010	L832	A826	K726			
LEU	G933	G933					
TYR	V934	S935	S829	E731			
GLY	S935	S936	A830				
G1014	S936						M446
S1015	I941		Q833	D735	S632		N453
S1016	Q942		L834	K737	V633		
Y1017	G943		I835	L738	M547		L458
V1018	I944		L836		F548		V459
D1019	F945		P837	D741	N554		I462
F1020	N946		V845	S742			C463
L1021	P947		Y846	L745			E464
C1022	S948			I746	Q641		E465
C1023	P949			Q747	V643		L466
V1024	F950		C854		D644		K467
H1025	A851				V645		T468
K1026	H952		L857		A646		M469
E1027	I953		S858	L751	S647		L470
I1028			R859	Q758			E471
C1029							

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.177 , 0.253 0.199 , 0.256	Depositor DCC
R_{free} test set	1985 reflections (7.96%)	wwPDB-VP
Wilson B-factor (Å ²)	82.7	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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:HG3	1:A:311:ARG:HH21	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:OD1	2:B:492:ASN:O	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:O	2:B:861:GLU:HG3	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:O	2:B:617:ASN:ND2	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:HD12	1:A:749:LEU:O	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:O	2:B:493:LYS:CG	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:469:MET:CE	2:B:679:ARG:HA	2.17	0.74
2:B:1024:VAL:HG12	2:B:1028:ILE:CD1	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:60:LEU:HB3	1:A:67:ARG:NH1	2.04	0.71
1:A:673:GLN:HB3	1:A:685:LEU:HD12	1.72	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:HG3	1:A:311:ARG:NH2	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:406:ILE:O	2:B:406:ILE:CG2	2.43	0.65
2:B:1027:GLU:HA	2:B:1030:GLN:HB2	1.79	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:O	2:B:946:ASN:ND2	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:285:ARG:NH2	1:A:346:ASP:OD2	2.31	0.64
1:A:312:SER:OG	1:A:315:ASP:OD2	2.15	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:311:ARG:NH2	1:A:597:PRO:HB2	2.13	0.63
1:A:536:THR:HG22	1:A:537:GLU:H	1.61	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:314:ARG:NH1	2:B:782:GLU:OE2	2.33	0.62
2:B:386:CYS:SG	2:B:388:PHE:HD1	2.22	0.62
2:B:446:MET:HE1	2:B:578:LEU:HD13	1.81	0.62
2:B:1000:VAL:HG13	2:B:1001:PHE:N	2.14	0.62
2:B:946:ASN:O	2:B:946:ASN:CG	2.37	0.62
2:B:1032:LEU:HG	2:B:1033:ASN:N	2.15	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:HA	1:A:238:MET:CE	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:H	1:A:673:GLN:CD	2.03	0.60
2:B:861:GLU:O	2:B:861:GLU:CG	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:O	2:B:591:PRO:CG	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:992:LYS:HB3	2:B:996:GLN:HG3	1.87	0.57
2:B:996:GLN:HB3	2:B:997:PRO:CD	2.28	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:289:ARG:NH1	2:B:742:SER:O	2.38	0.57
2:B:442:ALA:HA	2:B:484:ILE:HG23	1.86	0.57
2:B:643:VAL:HG12	2:B:643:VAL:O	2.02	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:84:ALA:HB2	1:A:91:ARG:HD3	1.88	0.56
1:A:148:LYS:O	1:A:152:GLN:HG3	2.05	0.56
1:A:236:ILE:O	1:A:236:ILE:HG22	2.04	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
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:C	2:B:523:LEU:HD23	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:HH21	1:A:311:ARG:CG	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:OE1	1:A:413:GLU:N	2.29	0.54
1:A:313:TRP:CD1	1:A:592:VAL:O	2.60	0.54
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:121:VAL:CG2	1:A:494:ILE:HG13	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:519:GLN:OE1	1:A:576:LEU:HB2	2.08	0.54
1:A:556:LYS:HG2	1:A:557:PHE:CE2	2.43	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:60:LEU:HB3	1:A:67:ARG:HH11	1.73	0.52
1:A:239:ASN:N	1:A:239:ASN:HD22	2.06	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:NH2	1:A:311:ARG:CG	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:77:ASP:CG	1:A:79:ARG:O	2.49	0.51
1:A:476:ARG:HG2	1:A:502:ASN:OD1	2.10	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:HA	1:A:591:GLN:NE2	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:51:LEU:HD12	1:A:52:PRO:HD3	1.92	0.50
1:A:313:TRP:HA	1:A:316:ILE:HG22	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:77:ASP:OD1	1:A:79:ARG:O	2.29	0.49
1:A:426:LEU:HD21	1:A:447:LYS:HB2	1.93	0.49
2:B:322:CYS:SG	2:B:771:SER:C	2.90	0.49
2:B:363:ARG:CZ	2:B:370:TYR:CE1	2.83	0.49
2:B:365:ASN:N	2:B:393:ASN:OD1	2.44	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:C	1:A:700:PHE:CD1	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:78:TYR:HD1	1:A:101:ILE:HG12	1.77	0.49
1:A:389:VAL:O	1:A:389:VAL:CG1	2.61	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:O	2:B:600:LYS:HG3	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: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
2:B:1009:LYS:HG2	2:B:1016:SER:HB3	1.96	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:427:ALA:HB3	2:B:759:ARG:HB3	1.96	0.47
2:B:523:LEU:HD23	2:B:524:ASP:OD1	2.14	0.47
1:A:66:CYS:SG	1:A:88:CYS:SG	3.11	0.47
1:A:102:SER:HB3	1:A:105:ASN:CA	2.44	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: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:1025:HIS:HA	2:B:1028:ILE:HD12	1.96	0.47
1:A:102:SER:HB3	1:A:105:ASN:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:522:LEU:HD11	2:B:526:PHE:HB2	1.97	0.47
2:B:642:TYR:OH	2:B:644:ASP:OD2	2.31	0.47
1:A:169:PHE:CD1	1:A:169:PHE:C	2.88	0.47
2:B:462:ILE:O	2:B:466:LEU:HB2	2.15	0.47
2:B:547:MET:HB2	2:B:547:MET:HE3	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:HA	1:A:591:GLN:HE21	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:81:LYS:HE2	1:A:99:ALA:HA	1.98	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
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:O	2:B:286:THR:OG1	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:79:ARG:O	1:A:80:ALA:HB3	2.16	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: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:HA	1:A:33:ARG:HD3	1.73	0.45
1:A:652:THR:HG23	1:A:655:GLN:O	2.15	0.45
2:B:388:PHE:CD1	2:B:388:PHE:N	2.84	0.45
2:B:1022:CYS:O	2:B:1026:LYS:HG3	2.17	0.45
1:A:83:TRP:CE2	1:A:92:ASN:HB2	2.52	0.45
1:A:529:LEU:HD23	1:A:529:LEU:HA	1.88	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:35:VAL:CG1	1:A:549:GLN:HE21	2.29	0.44
1:A:254:VAL:HA	1:A:255:PRO:HD2	1.66	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: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
2:B:602:LEU:N	2:B:605:THR:CG2	2.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:829:SER:HB2	2:B:833:GLN:OE1	2.17	0.44
2:B:1032:LEU:O	2:B:1033:ASN:HB2	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: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
2:B:1000:VAL:CG1	2:B:1001:PHE:N	2.79	0.43
1:A:47:GLU:HG2	1:A:453:PRO:HB3	2.00	0.43
1:A:311:ARG:NE	1:A:359:GLU:OE2	2.49	0.43
1:A:60:LEU:CB	1:A:67:ARG:NH1	2.77	0.43
1:A:589:PHE:C	1:A:590:LEU:HD23	2.39	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:570:LYS:HE2	2:B:629:HIS:NE2	2.33	0.43
2:B:1024:VAL:CG1	2:B:1028:ILE:HD11	2.40	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:81:LYS:HZ1	1:A:99:ALA:HB1	1.84	0.43
1:A:370:TYR:CE2	1:A:389:VAL:HG13	2.46	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:3:THR:HG22	1:A:5:LEU:H	1.84	0.42
1:A:240:LEU:O	1:A:243:LEU:HB3	2.19	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:375:MET:SD	2:B:386:CYS:HA	2.59	0.42
2:B:1015:SER:HB2	2:B:1019:ASP:HB3	2.01	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:723:ASP:OD2	2:B:726:LYS:HE2	2.20	0.42
2:B:845:VAL:HG13	2:B:1017:TYR:CD1	2.55	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:374:PHE:CE2	2:B:745:LEU:HD22	2.56	0.41
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: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:73:LEU:HD11	1:A:500:ALA:HB2	2.00	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:CD1	1:A:568:PHE:C	2.93	0.41
1:A:656:ILE:HD13	1:A:656:ILE:HA	1.94	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:679:GLU:OE1	1:A:682:ARG:NH1	2.53	0.41
2:B:523:LEU:C	2:B:523:LEU:CD2	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:17:VAL:HG13	1:A:19:PHE:CD1	2.56	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
1:A:658:ILE:HD12	1:A:705:TYR:OH	2.20	0.41
2:B:441:PRO:HG2	2:B:484:ILE:HG12	2.02	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:443:PHE:HB3	2:B:579:PHE:CE2	2.56	0.40
2:B:492:ASN:OD1	2:B:492:ASN:C	2.53	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:334:LEU:H	2:B:334:LEU:HD22	1.86	0.40
2:B:651:VAL:O	2:B:655:THR:HB	2.21	0.40
2:B:787:ILE:HD13	2:B:787:ILE:HA	1.80	0.40
2:B:845:VAL:HG22	2:B:1017:TYR:CE1	2.55	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:475:LYS:HG3	2:B:475:LYS:O	2.21	0.40
2:B:1032:LEU:O	2:B:1033:ASN:CB	2.69	0.40
1:A:190:ARG:NH1	2:B:517:GLU:O	2.54	0.40
1:A:745:ASP:O	1:A:746:ASP:C	2.58	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%)	30	60
2	B	763/770 (99%)	718 (94%)	39 (5%)	6 (1%)	16	44
All	All	1471/1535 (96%)	1384 (94%)	78 (5%)	9 (1%)	22	50

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%)	29	54
2	B	672/682 (98%)	645 (96%)	27 (4%)	27	52
All	All	1296/1348 (96%)	1246 (96%)	50 (4%)	27	53

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

Sometimes 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 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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	716/765 (93%)	-0.39	7 (0%) 79 71	26, 71, 129, 225	0
2	B	767/770 (99%)	-0.35	10 (1%) 74 66	31, 74, 160, 275	0
All	All	1483/1535 (96%)	-0.37	17 (1%) 77 70	26, 72, 149, 275	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	742	ILE	5.0
1	A	741	PRO	3.8
2	B	1015	SER	3.0
2	B	857	LEU	2.9
2	B	523	LEU	2.7
1	A	700	PHE	2.5
2	B	830	ALA	2.5
1	A	746	ASP	2.5
2	B	997	PRO	2.5
2	B	3	GLY	2.4
2	B	469	MET	2.4
2	B	902	MET	2.4
2	B	960	LEU	2.2
1	A	4	TYR	2.2
1	A	593	PHE	2.2
1	A	52	PRO	2.2
2	B	967	TYR	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ZN	B	1101	1/1	0.89	0.10	81,81,81,81	0
3	ZN	A	801	1/1	0.96	0.10	70,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.