



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2017 – 07:08 PM EDT

PDB ID : 5KYY
Title : Crystal structure of Sec23 and TANGO1 peptide4 complex
Authors : Ma, W.; Goldberg, J.
Deposited on : unknown
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

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20029824

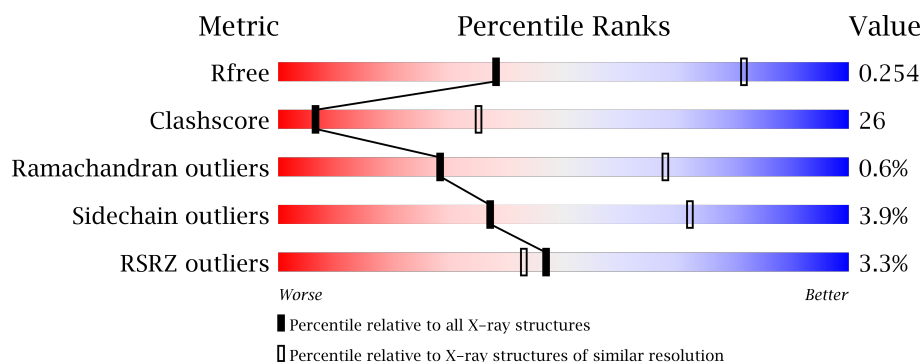
1 Overall quality at a glance

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}	100719	1679 (3.50-3.30)
Clashscore	112137	1832 (3.50-3.30)
Ramachandran outliers	110173	1789 (3.50-3.30)
Sidechain outliers	110143	1789 (3.50-3.30)
RSRZ outliers	101464	1709 (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 ≥ 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>58%</div> <div>34%</div> <div>6%</div> </div>
2	B	770	<div> <div>4%</div> <div>58%</div> <div>39%</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).

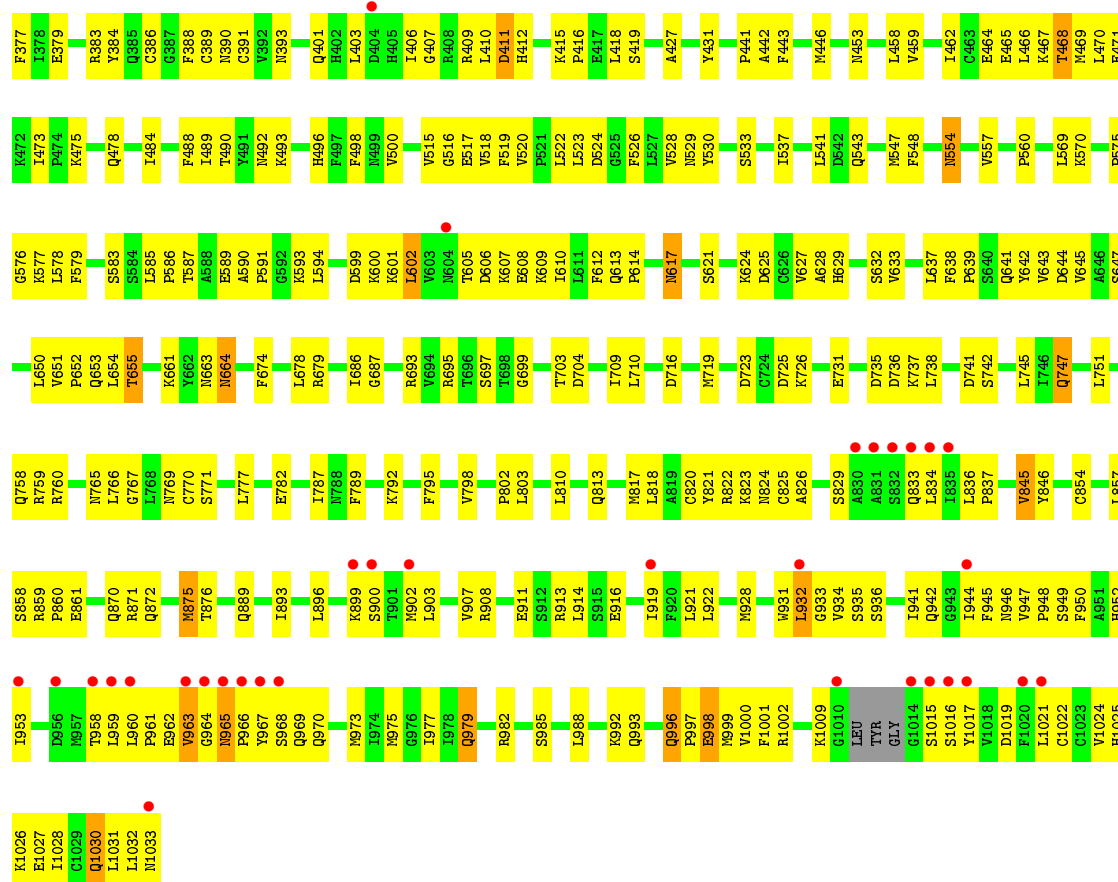
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

These plots are drawn for all protein, RNA and DNA 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.

- Chain A:

Sequence logo for Chain A. The y-axis lists amino acids: MET, THR, T3, Y4, L5, D15, G16, V17, R18, F19, S20, K21, N22, V23, Y24, P25, R33, K34, V35, P44, L45, E47, L51, P52, P53, L54, Q55, Y56, E57, P58, V59, L60, C61, C66, R67, N71, P72, L73, D77, V78, R79, C80, K81, L82, L83, A84, C85, C88, Y89, R90. The x-axis shows sequence positions from 1 to 200. The logo height at each position indicates the information content. A color scale at the top indicates the probability of each amino acid at that position, ranging from 2% (red) to 6% (yellow).

- Chain B:
-
- 4% 58% 39%
- Chain B states (from left to right): M1, M2, S278, S279, G280, G281, G282, G283, G284, G285, T286, G289, G290, Q291, V296, C300, M301, I302, Q303, D304, Q305, G306, N307, P310, I313, R314, T317, Y318, C319, C322, I334, I338, S346, N347, V354, S359, R363, C364, N365, R366, Y370, F374, M375, S376.



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	3.20 (at 3.40Å)	Xtriage
Refinement program	PHENIX 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 ²)	82.4	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 53.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	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 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: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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	708/765 (92%)	666 (94%)	39 (6%)	3 (0%)	38	75
2	B	763/770 (99%)	718 (94%)	39 (5%)	6 (1%)	22	62
All	All	1471/1535 (96%)	1384 (94%)	78 (5%)	9 (1%)	28	68

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 [i](#)

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%)	39	73
2	B	672/682 (98%)	645 (96%)	27 (4%)	36	71
All	All	1296/1348 (96%)	1246 (96%)	50 (4%)	37	72

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, 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%)	0.01	15 (2%) 64 60	26, 71, 129, 225	0
2	B	767/770 (99%)	0.10	34 (4%) 35 32	31, 74, 160, 275	0
All	All	1483/1535 (96%)	0.06	49 (3%) 47 43	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, 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	LLDF	B-factors(\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.