



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2017 – 10:30 PM EST

PDB ID : 5T4Y
Title : Crystal structure of BT1762-1763
Authors : van den Berg, B.
Deposited on : 2016-08-30
Resolution : 3.10 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
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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-20028442

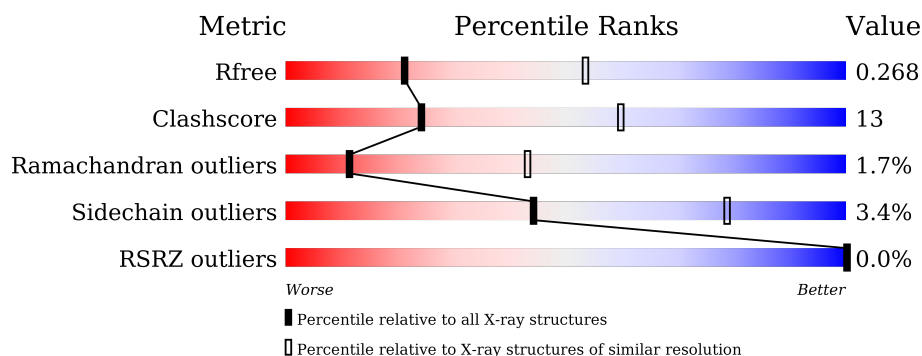
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	576	<div> <div>76%</div> <div>19%</div> <div>• •</div> </div>
1	B	576	<div> <div>76%</div> <div>20%</div> <div>• •</div> </div>
2	C	1041	<div> <div>48%</div> <div>27%</div> <div>•</div> <div>22%</div> </div>
2	D	1041	<div> <div>48%</div> <div>27%</div> <div>•</div> <div>22%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21727 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 SusD homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	2	0
			4450	2818	737	874	21			
1	B	553	Total	C	N	O	S	0	2	0
			4460	2824	740	875	21			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	553	HIS	-	expression tag	UNP Q8A6W4
A	554	HIS	-	expression tag	UNP Q8A6W4
A	555	HIS	-	expression tag	UNP Q8A6W4
A	556	HIS	-	expression tag	UNP Q8A6W4
A	557	HIS	-	expression tag	UNP Q8A6W4
A	558	HIS	-	expression tag	UNP Q8A6W4
B	553	HIS	-	expression tag	UNP Q8A6W4
B	554	HIS	-	expression tag	UNP Q8A6W4
B	555	HIS	-	expression tag	UNP Q8A6W4
B	556	HIS	-	expression tag	UNP Q8A6W4
B	557	HIS	-	expression tag	UNP Q8A6W4
B	558	HIS	-	expression tag	UNP Q8A6W4

- Molecule 2 is a protein called SusC homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	807	Total	C	N	O	S	0	0	0
			6406	4057	1089	1241	19			
2	C	807	Total	C	N	O	S	0	0	0
			6406	4057	1089	1241	19			

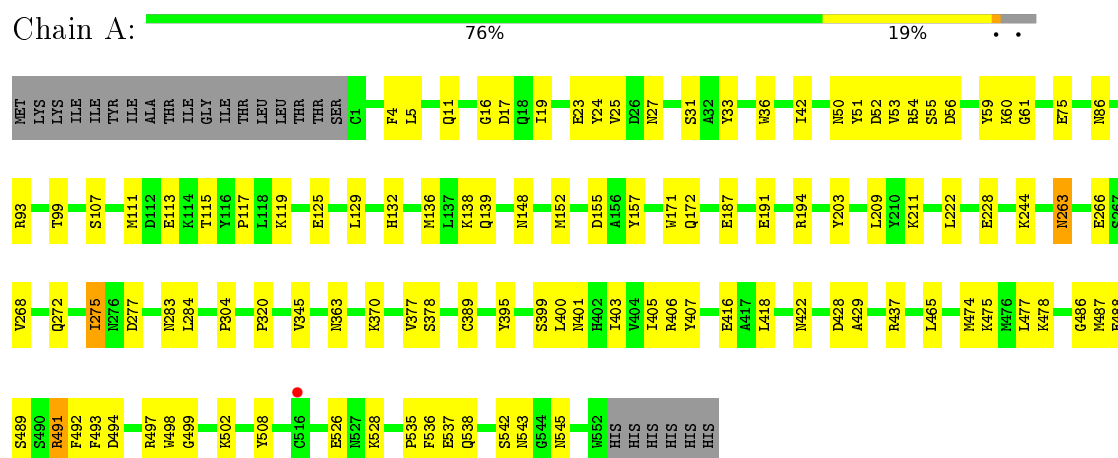
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total 2	Mg 2	0	0
3	A	2	Total 2	Mg 2	0	0
3	C	1	Total 1	Mg 1	0	0

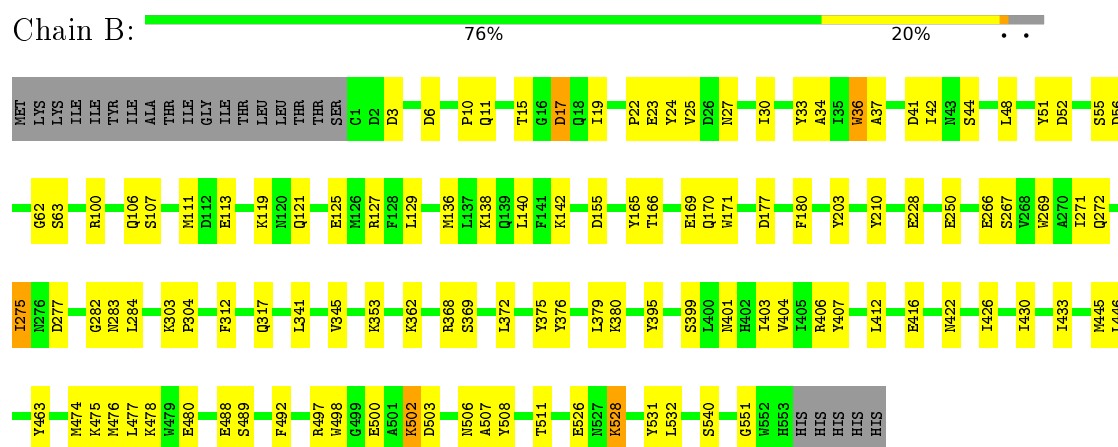
3 Residue-property plots

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.

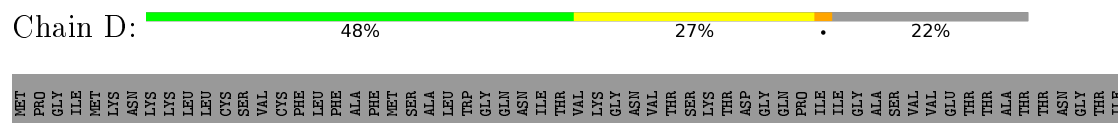
• Molecule 1: SusD homolog



• Molecule 1: SusD homolog



• Molecule 2: SusC homolog



T1009	L911	D817	S703	E604	R502	G403	K318
L912	E818	L704	L705	M605	G503	D406	E319
N913	H822	H706	G706	K608	H505	R407	S320
A914	A823	S707	L708	D614	H506	R408	S321
P925	T824	E709	E709	D615	L507	M409	F322
A926	Q825	E712	E712	L616	D516	P410	L325
L927	E826	G827	G827	L617	S520	R411	
T928	A828	A828	A828	L618	S520	E415	Y328
N933	R832	R832	R832	Q624	D525	Y422	L331
N934	E833	E833	E833	Q628	L528	M425	L334
E935	R834	R834	R834	L529	L529	R426	K335
Q936	Y835	Y835	Y835	G632	T530	M427	D336
R937	R836	R836	R836	L633	Y533	F428	T337
V938	D837	D837	D837	T637	G429	D430	D338
V939	L838	L838	L838	L638	H534	A431	
T940				Y639	H535	Y432	R345
V943	D845	D845	D845	A640	G541	V433	R346
K950	E846	E846	E846	N642	Y546	N434	D349
L951	R847	R847	R847	N642	G547	L435	Y350
	Q849	Q849	Q849	D647	L546	T436	K351
Q955	N850	N850	N850	S648	G549	P437	L352
L956	H851	H851	H851	G651	Y562	F438	L353
S965	L852	L852	L852	T656	S564	K439	D354
K966	P857	P857	P857	A657	Y563	G440	D355
	L865	L865	L865	Y658	S564	F441	L356
R969	F872	F872	F872	I660	Y569	M442	L357
H970	D873	D873	D873	L669	T574	L449	G360
D971	T874	T874	T874	P670	L575	D450	H361
L973	T875	T875	T875	F673	R576	Y451	H362
R974	V884	V884	V884	K674	R577	K454	F363
	D885	D885	D885	R675	D578	Q455	T364
C977	L887	L887	L887	N676		A456	R367
N981	S888	S888	S888	Q677	Y582	P462	E370
L982	V890	V890	V890	I678	K585	Y463	V371
K986	K891	K891	K891	G679	H586	G466	P374
S987	K892	K892	K892	N682	H587	T467	G375
K988	S893	S893	S893	I683	K588	Q468	G376
N989	S894	S894	S894	N684	Y589	T469	I377
F990	D895	D895	D895	W685	A590	N470	I378
T991	N901	N901	N901	T691	P593	M471	E379
G992	V902	V902	V902	L695	S594	G472	D383
E993	F904	F904	F904	D696	L597	W483	
	L905	L905	L905	G697	G598	M487	V390
	N906	N906	N906	T697	L699	E497	S396
	K907	K907	K907	K701	T602	V498	I397
	G908	G908	G908	Q702		G499	
V1006	T909	T909	T909			K500	P400
N1007	R910	R910	R910			V401	
I1008						H501	G402

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.83Å 152.09Å 253.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	130.35 – 3.10 130.35 – 2.99	Depositor EDS
% Data completeness (in resolution range)	98.9 (130.35-3.10) 98.6 (130.35-2.99)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.198 , 0.270 0.194 , 0.268	Depositor DCC
R_{free} test set	3942 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	68.3	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 56.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21727	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.85% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.44	0/4562	0.62	2/6190 (0.0%)
1	B	0.49	1/4573 (0.0%)	0.66	1/6205 (0.0%)
2	C	0.59	8/6571 (0.1%)	0.76	4/8909 (0.0%)
2	D	0.52	0/6571	0.76	3/8909 (0.0%)
All	All	0.52	9/22277 (0.0%)	0.71	10/30213 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	709	GLU	CG-CD	-6.93	1.41	1.51
2	C	565	TYR	CE1-CZ	-6.63	1.29	1.38
2	C	565	TYR	CE2-CZ	-6.15	1.30	1.38
2	C	565	TYR	CG-CD1	-6.06	1.31	1.39
1	B	36	TRP	CB-CG	-5.99	1.39	1.50
2	C	565	TYR	CG-CD2	-5.97	1.31	1.39
2	C	977	CYS	CB-SG	-5.38	1.73	1.81
2	C	709	GLU	CD-OE1	-5.30	1.19	1.25
2	C	262	ASN	CA-CB	5.18	1.66	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	911	LEU	CA-CB-CG	6.11	129.35	115.30
2	D	911	LEU	CB-CG-CD2	5.82	120.89	111.00
1	A	275	ILE	CG1-CB-CG2	-5.81	98.62	111.40
2	D	449	LEU	CA-CB-CG	5.42	127.77	115.30
2	C	565	TYR	CA-CB-CG	5.39	123.65	113.40
2	C	449	LEU	CA-CB-CG	5.37	127.65	115.30
1	B	275	ILE	CG1-CB-CG2	-5.34	99.66	111.40
1	A	465	LEU	CB-CG-CD2	-5.20	102.16	111.00
2	D	911	LEU	CA-CB-CG	5.17	127.18	115.30
2	C	357	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	317	GLU	Peptide
2	D	353	ILE	Peptide
2	D	470	ASN	Peptide
2	D	584	GLY	Peptide

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	4450	0	4219	80	0
1	B	4460	0	4227	81	0
2	C	6406	0	6058	208	0
2	D	6406	0	6058	222	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
All	All	21727	0	20562	549	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 13.

All (549) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:427:MET:CE	2:C:427:MET:SD	2.35	1.12
2:D:427:MET:HE2	2:C:427:MET:SD	1.95	1.04
2:D:427:MET:HE3	2:C:427:MET:SD	2.00	1.00
1:B:275:ILE:HG22	1:B:284:LEU:HD11	1.47	0.95
2:D:365:LEU:HD13	2:D:427:MET:SD	2.12	0.90
2:C:986:LYS:HD2	2:C:986:LYS:H	1.38	0.87
1:A:55:SER:HB3	1:A:492:PHE:HB2	1.59	0.84
2:C:873:ASP:OD2	2:C:974:ARG:NH2	2.11	0.83
2:C:832:ARG:NH1	2:C:935:GLU:OE2	2.12	0.81
2:C:243:GLN:O	2:C:247:ASN:OD1	1.99	0.81
2:C:232:LEU:H	2:C:906:ASN:HD21	1.27	0.81
2:C:434:ASN:HD21	2:C:442:ASN:HD22	1.28	0.80
2:D:352:LEU:HD12	2:D:357:LEU:HD13	1.63	0.78
2:C:520:SER:HB3	2:C:546:TYR:HB2	1.65	0.78
2:D:793:VAL:HG11	2:D:849:GLN:HE21	1.49	0.77
2:C:568:ARG:NH2	2:C:603:GLN:O	2.18	0.77
2:D:832:ARG:NH1	2:D:935:GLU:OE2	2.17	0.77
2:D:619:ARG:NH1	2:D:696:ASP:OD2	2.18	0.76
2:C:605:ASN:HA	2:C:608:LYS:HE3	1.66	0.75
2:C:462:PRO:HB3	2:C:472:GLY:HA2	1.67	0.75
1:B:113:GLU:HG3	1:B:119:LYS:HD3	1.66	0.75
1:A:275:ILE:HG23	1:A:399:SER:HB3	1.67	0.75
2:C:832:ARG:NH2	2:C:926:ALA:O	2.18	0.74
1:B:63:SER:HB3	2:C:904:PHE:CE2	2.23	0.74
2:D:568:ARG:HG2	2:D:603:GLN:HB3	1.69	0.73
1:B:478:LYS:NZ	1:B:500:GLU:OE2	2.15	0.72
2:D:825:GLN:HB3	2:D:828:ALA:HB2	1.72	0.71
1:B:282:GLY:HA2	1:B:284:LEU:HD13	1.70	0.71
1:B:42:ILE:HD13	1:B:395:TYR:CE2	2.26	0.70
2:D:963:VAL:HG13	2:D:964:ILE:HG23	1.71	0.70
1:B:528:LYS:HE2	1:B:551:GLY:O	1.92	0.70
2:C:383:ASP:HB3	2:C:893:LYS:HZ1	1.56	0.70
2:D:504:ASP:HB2	2:D:562:ASN:HB2	1.72	0.70
2:C:742:LYS:HE3	2:C:776:LEU:HD21	1.75	0.69
2:D:825:GLN:HG3	2:D:844:ILE:HG13	1.75	0.69
1:A:25:VAL:HG22	1:A:107:SER:HB3	1.73	0.69
2:C:506:MET:HG2	2:C:507:ILE:N	2.08	0.69
1:A:272:GLN:OE1	1:A:401:ASN:ND2	2.22	0.68
1:A:5:LEU:HD12	2:D:588:ARG:HD3	1.74	0.68
2:C:298:GLU:HG2	2:C:390:VAL:HG21	1.76	0.68
2:C:237:TYR:OH	2:C:904:PHE:HB3	1.94	0.68
1:B:56:ASP:HA	1:B:508:TYR:CE2	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:607:MET:O	2:D:609:GLU:N	2.26	0.67
2:D:810:ASP:OD2	2:D:836:ARG:HB3	1.94	0.67
2:C:304:VAL:HG12	2:C:331:LEU:HB2	1.77	0.67
2:C:674:LYS:HE2	2:C:676:ASN:OD1	1.95	0.67
1:B:55:SER:HB3	1:B:492:PHE:HB2	1.76	0.66
2:C:850:ASN:O	2:C:852:ILE:HG23	1.96	0.66
1:A:172:GLN:OE1	1:A:211:LYS:NZ	2.28	0.66
2:C:504:ASP:HB2	2:C:562:ASN:HB2	1.78	0.65
2:D:760:LEU:HD12	2:D:869:TYR:HB2	1.77	0.64
2:C:266:ASN:HB3	2:C:272:VAL:CG2	2.28	0.64
2:C:637:THR:HG22	2:C:678:ILE:HA	1.79	0.64
2:D:902:VAL:HG23	2:D:905:LEU:HD11	1.78	0.64
2:C:528:ILE:HG22	2:C:530:THR:HG22	1.79	0.64
2:C:374:PRO:HD2	2:C:377:ILE:HG13	1.78	0.64
1:A:275:ILE:CG2	1:A:399:SER:HB3	2.27	0.64
2:D:705:TYR:CZ	2:D:751:GLY:HA3	2.32	0.64
2:C:383:ASP:HB3	2:C:893:LYS:NZ	2.13	0.64
2:C:987:SER:O	2:C:989:ASN:N	2.31	0.63
2:D:334:ILE:HD11	2:D:378:ILE:HD11	1.80	0.63
1:A:19:ILE:HG13	2:D:639:TYR:CD2	2.34	0.63
2:D:794:LYS:HB2	2:D:805:VAL:HG21	1.80	0.63
2:D:301:ARG:HG3	2:D:335:LYS:HG2	1.80	0.63
2:D:453:ASN:OD1	2:D:480:GLN:NE2	2.29	0.63
1:B:275:ILE:HG22	1:B:284:LEU:CD1	2.27	0.62
2:C:282:LEU:HG	2:C:290:VAL:HG22	1.80	0.62
2:C:993:GLU:OE2	2:C:993:GLU:HA	1.97	0.62
1:A:535:PRO:HG2	1:A:538:GLN:HB2	1.81	0.62
2:D:377:ILE:HD13	2:D:414:LEU:HD21	1.82	0.62
2:C:221:SER:HB3	2:C:305:ILE:HB	1.81	0.62
1:A:125:GLU:OE1	1:A:194:ARG:NH2	2.29	0.62
2:C:601:ILE:HG21	2:C:616:LEU:HD23	1.81	0.62
2:C:810:ASP:OD2	2:C:836:ARG:HB3	2.00	0.62
1:B:416:GLU:CD	1:B:497:ARG:HH21	2.02	0.62
2:C:582:ARG:HD2	2:C:632:ASN:HA	1.83	0.61
2:C:593:PRO:HD2	2:C:624:GLN:HG3	1.83	0.61
1:A:138:LYS:HG2	1:A:171:TRP:CH2	2.36	0.61
1:A:24:TYR:O	1:A:27:ASN:HB2	2.01	0.61
2:C:301:ARG:HG3	2:C:335:LYS:HG2	1.82	0.60
2:C:818:GLU:O	2:C:822:HIS:HB2	2.01	0.60
2:D:365:LEU:CD1	2:D:427:MET:SD	2.87	0.60
2:C:886:ILE:HD13	2:C:998:PRO:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:682:ASN:ND2	2:C:682:ASN:O	2.35	0.59
2:D:370:GLU:HB3	2:D:422:TYR:CE2	2.37	0.59
1:B:33:TYR:OH	1:B:125:GLU:OE1	2.15	0.59
2:C:232:LEU:HD22	2:C:907:LYS:O	2.02	0.59
2:D:279:SER:O	2:D:281:TYR:N	2.33	0.59
2:D:682:ASN:ND2	2:D:682:ASN:O	2.36	0.59
2:C:295:TRP:CZ3	2:C:410:PRO:HD2	2.35	0.59
1:B:445:MET:HG2	1:B:446:LEU:HG	1.85	0.59
1:A:502:LYS:HG3	1:A:526:GLU:HB2	1.84	0.58
1:B:25:VAL:HG21	1:B:111:MET:SD	2.43	0.58
1:A:536:PHE:HZ	2:D:793:VAL:HG13	1.68	0.58
1:B:416:GLU:OE1	1:B:497:ARG:NH2	2.36	0.58
2:D:637:THR:HG23	2:D:679:GLY:H	1.68	0.58
2:D:986:LYS:HD2	2:D:990:PHE:HD2	1.67	0.58
2:D:214:ILE:HG12	2:C:352:LEU:HD22	1.85	0.58
1:A:42:ILE:HD13	1:A:395:TYR:CE2	2.38	0.58
2:C:791:ASN:HD21	2:C:804:GLN:CG	2.16	0.58
2:D:793:VAL:HG11	2:D:849:GLN:NE2	2.18	0.58
1:B:30:ILE:HG21	2:C:670:PRO:HB2	1.84	0.58
2:C:832:ARG:NH2	2:C:928:THR:HG23	2.19	0.58
2:C:894:SER:HA	2:C:908:GLY:HA3	1.85	0.57
2:D:962:ALA:O	2:D:966:LYS:HG3	2.03	0.57
2:D:233:ASN:HB2	2:D:236:GLN:OE1	2.05	0.57
2:D:618:LEU:HD23	2:D:695:ILE:HG13	1.86	0.57
1:A:51:TYR:OH	1:A:86:ASN:O	2.23	0.57
2:D:613:LEU:HD12	2:D:699:LEU:HD22	1.85	0.57
2:C:422:TYR:CG	2:C:454:LYS:HD2	2.39	0.57
2:C:691:THR:HG23	2:C:712:TYR:HB3	1.86	0.57
1:B:210:TYR:HA	1:B:497:ARG:HD2	1.86	0.57
2:D:610:LEU:O	2:D:611:THR:HG22	2.05	0.56
1:A:60:LYS:NZ	1:A:61:GLY:O	2.38	0.56
2:C:825:GLN:HB3	2:C:828:ALA:HB2	1.87	0.56
2:C:648:SER:HB3	2:C:651:GLY:O	2.05	0.56
1:B:34:ALA:O	1:B:37:ALA:N	2.39	0.56
2:D:587:HIS:CD2	2:D:684:LYS:HB3	2.41	0.56
2:C:739:GLY:HA3	2:C:777:GLU:O	2.06	0.56
2:D:766:GLY:HA2	2:D:863:LEU:HA	1.86	0.56
1:A:25:VAL:HG21	1:A:111:MET:SD	2.46	0.56
1:A:50:ASN:O	1:A:53:VAL:HG22	2.06	0.56
2:C:642:ASN:O	2:C:656:THR:OG1	2.20	0.56
2:C:832:ARG:HB3	2:C:933:ASN:ND2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:MET:HB3	1:A:157:TYR:CE2	2.40	0.55
2:C:748:PHE:HB3	2:C:768:ILE:HG23	1.88	0.55
2:D:336:ASP:OD2	2:D:411:ARG:NH2	2.39	0.55
2:D:420:ASN:HB3	2:D:458:TYR:CD1	2.41	0.55
1:A:377:VAL:HG12	1:A:378:SER:O	2.06	0.55
1:A:418:LEU:HB2	1:A:429:ALA:HB2	1.89	0.55
2:D:561:MET:O	2:D:572:SER:HA	2.07	0.55
2:C:298:GLU:O	2:C:335:LYS:NZ	2.39	0.55
2:C:436:THR:HG23	2:C:442:ASN:HB3	1.89	0.55
2:C:817:ASP:OD1	2:C:818:GLU:N	2.39	0.55
2:D:394:ASP:OD1	2:D:394:ASP:N	2.37	0.55
2:D:835:TYR:CZ	2:D:937:ARG:HD3	2.41	0.55
1:B:275:ILE:HG23	1:B:399:SER:HB3	1.89	0.55
1:B:6:ASP:OD2	2:C:588:ARG:NH2	2.39	0.55
2:D:400:PRO:O	2:D:466:GLY:HA3	2.06	0.55
2:D:498:VAL:HG12	2:D:498:VAL:O	2.06	0.55
2:D:776:LEU:O	2:D:797:VAL:HG13	2.06	0.55
2:D:637:THR:HG22	2:D:678:ILE:HA	1.88	0.55
2:D:318:LYS:HD2	2:C:212:ILE:HG13	1.87	0.55
1:A:113:GLU:CG	1:A:119:LYS:HD3	2.37	0.54
1:B:138:LYS:HG2	1:B:171:TRP:CZ2	2.41	0.54
2:D:835:TYR:CE1	2:D:937:ARG:HD3	2.42	0.54
2:C:965:SER:O	2:C:970:MET:HB2	2.08	0.54
1:A:56:ASP:OD1	1:A:56:ASP:N	2.41	0.54
2:C:914:ALA:HB1	2:C:925:PRO:O	2.08	0.54
2:D:808:ILE:HA	2:D:940:THR:HG23	1.90	0.54
2:C:875:THR:HG23	2:C:955:GLN:HB3	1.89	0.54
1:A:113:GLU:HG2	1:A:119:LYS:HD3	1.88	0.54
2:C:500:LYS:HG2	2:C:565:TYR:HB3	1.89	0.53
1:A:138:LYS:HG2	1:A:171:TRP:CZ2	2.43	0.53
1:A:543:ASN:ND2	2:D:780:GLU:HB2	2.23	0.53
2:C:497:GLU:OE2	2:C:502:ARG:HB3	2.08	0.53
2:C:528:ILE:HB	2:C:533:TYR:CG	2.43	0.53
2:C:981:ASN:O	2:C:1006:VAL:HG22	2.08	0.53
2:D:574:THR:OG1	2:D:594:SER:HB3	2.08	0.53
1:A:31:SER:HB2	2:D:672:GLY:HA3	1.90	0.53
2:C:353:ILE:HG22	2:C:356:ILE:HB	1.90	0.53
2:D:791:ASN:HD21	2:D:804:GLN:HG2	1.74	0.53
2:C:228:LYS:HD3	2:C:296:PHE:CG	2.43	0.53
2:D:993:GLU:HA	2:D:993:GLU:OE2	2.09	0.53
2:C:585:LYS:HA	2:C:588:ARG:HG3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:420:ASN:HB3	2:D:458:TYR:HD1	1.74	0.53
2:D:613:LEU:HD12	2:D:699:LEU:CD2	2.39	0.53
2:D:747:GLU:OE1	2:D:767:ASN:ND2	2.42	0.53
1:B:24:TYR:O	1:B:27:ASN:HB2	2.08	0.53
2:C:231:VAL:HB	2:C:906:ASN:ND2	2.24	0.53
2:C:605:ASN:HA	2:C:608:LYS:CE	2.39	0.53
1:A:23:GLU:N	1:A:23:GLU:OE1	2.24	0.52
2:C:951:LEU:O	2:C:951:LEU:HD23	2.09	0.52
1:B:121:GLN:O	1:B:125:GLU:HG3	2.09	0.52
2:D:652:GLN:HB3	2:D:654:TYR:HE1	1.75	0.52
1:B:10:PRO:HB3	2:C:633:LEU:HD23	1.91	0.52
2:C:360:GLY:HA3	2:C:432:TYR:CZ	2.45	0.52
2:D:807:TYR:CD2	2:D:937:ARG:HG3	2.45	0.52
2:C:376:GLY:HA2	2:C:379:GLU:OE1	2.09	0.52
2:C:845:ASP:OD2	2:C:847:ARG:HG3	2.10	0.52
2:D:415:GLU:O	2:D:418:LYS:HG2	2.09	0.52
1:B:303:LYS:HE3	1:B:376:TYR:O	2.10	0.52
2:C:280:LYS:HB3	2:C:281:TYR:CD1	2.44	0.52
2:D:255:ASN:HD21	2:D:259:TYR:HB2	1.74	0.52
2:D:678:ILE:HD11	2:D:728:LEU:HD21	1.91	0.52
1:A:23:GLU:HG2	1:A:24:TYR:CD1	2.44	0.52
2:C:616:LEU:HD12	2:C:697:PHE:HB3	1.92	0.52
1:B:36:TRP:NE1	1:B:129:LEU:HD22	2.25	0.52
2:C:345:ARG:C	2:C:346:MET:HG3	2.30	0.52
1:A:370:LYS:HG3	2:D:256:ALA:HA	1.91	0.52
2:D:232:LEU:HD22	2:D:907:LYS:O	2.09	0.51
2:C:578:ASP:O	2:C:589:TYR:HA	2.11	0.51
2:D:241:MET:CE	2:D:255:ASN:HD22	2.24	0.51
2:D:780:GLU:CD	2:D:780:GLU:H	2.13	0.51
1:B:48:LEU:HD22	1:B:140:LEU:HD11	1.92	0.51
2:C:872:PHE:HD2	2:C:956:LEU:HD21	1.75	0.51
2:C:362:HIS:HB2	2:C:430:ASP:OD1	2.10	0.51
2:C:483:TRP:HA	2:C:516:ASP:HB3	1.93	0.51
2:C:628:GLN:HB2	2:C:685:TRP:CZ3	2.46	0.51
2:C:731:GLY:O	2:C:733:SER:N	2.44	0.51
2:D:528:ILE:HB	2:D:533:TYR:CG	2.46	0.51
2:C:401:VAL:HA	2:C:467:THR:HG23	1.92	0.50
2:D:718:ILE:O	2:D:737:ASN:HA	2.10	0.50
2:D:435:LEU:O	2:D:437:PRO:HD3	2.10	0.50
1:A:5:LEU:CD1	2:D:588:ARG:HD3	2.39	0.50
1:B:403:ILE:HG21	1:B:406:ARG:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:279:SER:O	2:D:279:SER:OG	2.21	0.50
2:C:901:ASN:ND2	2:C:901:ASN:O	2.45	0.50
2:D:353:ILE:HG22	2:D:356:ILE:HB	1.93	0.50
2:D:854:ASP:OD1	2:D:856:THR:OG1	2.30	0.50
1:B:177:ASP:O	1:B:180:PHE:N	2.43	0.50
2:D:854:ASP:O	2:D:885:ASP:HB2	2.12	0.50
1:A:155:ASP:OD1	1:A:155:ASP:N	2.45	0.50
1:B:272:GLN:OE1	1:B:401:ASN:ND2	2.40	0.50
2:C:266:ASN:HB3	2:C:272:VAL:HG21	1.93	0.50
2:D:255:ASN:HD21	2:D:258:GLY:HA2	1.77	0.50
2:C:574:THR:OG1	2:C:594:SER:HB3	2.12	0.50
2:D:345:ARG:HG2	2:D:345:ARG:HH11	1.77	0.50
2:D:401:VAL:O	2:D:404:TRP:HD1	1.95	0.50
2:D:416:TYR:CE2	2:D:463:TYR:HB3	2.46	0.50
2:D:774:GLU:HA	2:D:799:HIS:O	2.12	0.50
2:C:568:ARG:HD2	2:C:569:TYR:CE2	2.47	0.49
1:B:540:SER:OG	2:C:792:GLY:O	2.30	0.49
2:C:808:ILE:HG23	2:C:836:ARG:HG2	1.94	0.49
2:D:652:GLN:HB3	2:D:654:TYR:CE1	2.47	0.49
1:A:152:MET:HB3	1:A:157:TYR:HE2	1.76	0.49
1:B:369:SER:HB2	1:B:372:LEU:HB3	1.93	0.49
2:C:336:ASP:OD2	2:C:411:ARG:NH2	2.45	0.49
2:D:547:GLY:O	2:C:535:TRP:HB3	2.11	0.49
2:D:824:THR:OG1	2:D:843:VAL:HG12	2.12	0.49
2:D:805:VAL:HG12	2:D:849:GLN:HG3	1.95	0.49
1:B:41:ASP:HB3	1:B:44:SER:OG	2.13	0.49
2:D:377:ILE:O	2:D:380:THR:HG22	2.13	0.49
2:D:691:THR:HG23	2:D:712:TYR:HB3	1.93	0.49
2:C:647:ASP:OD1	2:C:648:SER:N	2.45	0.49
2:D:258:GLY:HA2	2:D:259:TYR:HB2	1.94	0.49
2:D:705:TYR:HE1	2:D:753:ARG:HG2	1.77	0.49
1:B:507:ALA:O	1:B:511:THR:HG23	2.12	0.49
2:C:362:HIS:O	2:C:429:GLY:HA3	2.13	0.49
2:C:318:LYS:O	2:C:351:LYS:HB2	2.12	0.49
2:C:788:PHE:HD1	2:C:801:TYR:CE2	2.31	0.49
2:D:788:PHE:N	2:D:789:GLY:HA3	2.27	0.49
2:D:586:ASN:N	2:D:586:ASN:OD1	2.46	0.49
2:D:266:ASN:O	2:D:268:ASP:N	2.46	0.49
2:D:457:ARG:NH1	2:D:534:MET:O	2.46	0.48
2:D:339:PHE:HD2	2:D:370:GLU:HB2	1.78	0.48
2:D:506:MET:HG2	2:D:507:ILE:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:THR:O	1:A:117:PRO:HD3	2.14	0.48
2:D:449:LEU:HD22	2:C:425:TRP:HH2	1.79	0.48
1:A:542:SER:O	1:A:545:ASN:ND2	2.43	0.48
1:B:15:THR:O	1:B:17:ASP:N	2.47	0.48
2:C:905:LEU:HB2	2:C:907:LYS:HE2	1.94	0.48
2:D:293:THR:HG21	2:D:295:TRP:CE2	2.49	0.48
2:D:352:LEU:O	2:D:353:ILE:HG13	2.13	0.48
2:C:234:THR:HG22	2:C:292:ASP:CG	2.34	0.48
2:D:965:SER:O	2:D:970:MET:HB2	2.14	0.48
1:B:269:TRP:CZ3	1:B:404:VAL:HG21	2.49	0.48
2:C:218:ALA:HB3	2:C:1012:LEU:CD2	2.44	0.48
2:C:233:ASN:HB2	2:C:236:GLN:OE1	2.14	0.48
2:D:648:SER:HB3	2:D:651:GLY:O	2.14	0.48
2:D:891:LYS:HA	2:D:894:SER:OG	2.14	0.48
2:C:422:TYR:CD1	2:C:454:LYS:HD2	2.48	0.48
2:C:601:ILE:CG2	2:C:616:LEU:HD23	2.43	0.48
1:B:283:ASN:ND2	2:C:657:ALA:O	2.45	0.48
2:C:734:ARG:HG3	2:C:736:ILE:HG23	1.95	0.48
2:D:282:LEU:HD23	2:D:404:TRP:NE1	2.29	0.48
2:D:422:TYR:HA	2:D:456:ALA:HB2	1.95	0.48
2:D:613:LEU:CD1	2:D:699:LEU:HD22	2.44	0.48
1:A:363:ASN:OD1	1:A:363:ASN:N	2.47	0.47
1:B:52:ASP:CG	1:B:489:SER:HA	2.35	0.47
2:C:637:THR:CG2	2:C:679:GLY:H	2.26	0.47
2:D:953:ASN:ND2	2:D:979:ALA:O	2.38	0.47
2:D:397:TRP:HZ2	2:D:415:GLU:HG3	1.79	0.47
1:A:99:THR:OG1	2:D:729:GLY:HA3	2.14	0.47
2:D:902:VAL:CG2	2:D:905:LEU:HD11	2.43	0.47
2:C:252:PRO:O	2:C:255:ASN:ND2	2.41	0.47
2:C:902:VAL:HB	2:C:905:LEU:HD11	1.95	0.47
2:C:891:LYS:HA	2:C:894:SER:OG	2.15	0.47
2:C:906:ASN:C	2:C:907:LYS:HD2	2.35	0.47
1:A:478:LYS:HG2	1:A:498:TRP:CZ2	2.50	0.47
2:D:304:VAL:HG12	2:D:331:LEU:HB2	1.96	0.47
1:B:30:ILE:HG13	2:C:660:ILE:HG13	1.97	0.47
2:C:791:ASN:HD21	2:C:804:GLN:HG2	1.79	0.47
2:D:587:HIS:CD2	2:D:684:LYS:HD3	2.49	0.47
2:D:894:SER:O	2:D:910:ARG:HG3	2.14	0.47
1:B:19:ILE:HG13	2:C:639:TYR:CD2	2.50	0.47
2:D:383:ASP:HB2	2:D:905:LEU:HB3	1.97	0.47
2:D:364:THR:HB	2:D:428:PHE:CE1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:462:PRO:HB3	2:D:472:GLY:HA2	1.97	0.47
1:B:22:PRO:HA	1:B:25:VAL:HG23	1.97	0.47
1:B:502:LYS:HG2	1:B:506:ASN:HD21	1.80	0.47
2:C:857:PRO:HA	2:C:884:VAL:HG12	1.97	0.47
1:B:266:GLU:HG3	1:B:407:TYR:H	1.79	0.47
1:B:275:ILE:HG21	1:B:275:ILE:HD13	1.51	0.47
1:B:138:LYS:HE2	1:B:170:GLN:HB3	1.97	0.46
2:C:703:SER:O	2:C:752:TYR:HD1	1.98	0.46
1:A:263:ASN:HD21	1:A:401:ASN:ND2	2.14	0.46
1:B:380:LYS:NZ	1:B:488:GLU:OE2	2.47	0.46
2:C:886:ILE:HD11	2:C:990:PHE:HE1	1.81	0.46
2:D:878:TRP:CZ3	2:D:951:LEU:HB2	2.50	0.46
1:A:209:LEU:HD21	1:A:497:ARG:NE	2.29	0.46
1:A:56:ASP:HA	1:A:508:TYR:CE2	2.50	0.46
2:C:352:LEU:HD12	2:C:357:LEU:HD13	1.96	0.46
2:C:397:TRP:HZ2	2:C:415:GLU:HG3	1.80	0.46
2:C:525:ASP:HB2	2:C:541:GLY:H	1.81	0.46
2:D:289:PRO:HD3	2:D:393:SER:OG	2.16	0.46
2:D:441:PHE:HB2	2:D:494:TYR:CD1	2.50	0.46
2:D:576:ARG:HD3	2:D:578:ASP:OD1	2.15	0.46
2:C:422:TYR:HA	2:C:456:ALA:HB2	1.95	0.46
2:C:408:ARG:HG3	2:C:468:GLN:HG2	1.97	0.46
1:B:502:LYS:O	1:B:506:ASN:ND2	2.47	0.46
2:C:262:ASN:O	2:C:274:TYR:HB2	2.14	0.46
2:D:525:ASP:HB2	2:D:541:GLY:H	1.79	0.46
1:B:304:PRO:HG2	1:B:345:VAL:HG13	1.98	0.46
1:B:312:PHE:CG	1:B:341:LEU:HB2	2.50	0.46
2:C:791:ASN:N	2:C:791:ASN:HD22	2.13	0.46
2:D:280:LYS:HG2	2:D:281:TYR:CE1	2.51	0.46
2:D:404:TRP:HB3	2:D:405:PRO:HD2	1.96	0.46
1:A:275:ILE:HG21	1:A:275:ILE:HD13	1.69	0.46
2:C:530:THR:HG23	2:C:533:TYR:H	1.80	0.46
2:D:255:ASN:HD21	2:D:259:TYR:CB	2.28	0.46
2:D:459:PHE:CZ	2:D:531:PRO:HB3	2.50	0.46
2:D:950:LYS:NZ	2:D:996:GLU:OE2	2.45	0.46
1:A:55:SER:HB2	1:A:491:ARG:HG3	1.97	0.46
1:B:433:ILE:HG23	1:B:480:GLU:HG2	1.99	0.46
2:C:258:GLY:HA2	2:C:259:TYR:O	2.16	0.46
2:C:891:LYS:HE3	2:C:991:THR:HG21	1.98	0.46
2:D:599:TRP:CE2	2:D:601:ILE:HG12	2.51	0.45
2:D:690:GLN:OE1	2:D:713:LYS:HE3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:GLY:O	1:A:488:GLU:N	2.50	0.45
2:C:822:HIS:CG	2:C:823:ALA:H	2.33	0.45
2:C:400:PRO:O	2:C:466:GLY:HA3	2.17	0.45
2:D:315:GLY:HA2	2:D:320:SER:HB3	1.98	0.45
2:D:340:ASP:OD1	2:D:369:SER:HB3	2.17	0.45
2:D:586:ASN:ND2	2:D:587:HIS:ND1	2.65	0.45
1:B:15:THR:C	1:B:17:ASP:H	2.20	0.45
1:B:250:GLU:HG2	1:B:266:GLU:HB2	1.99	0.45
2:C:305:ILE:HD13	2:C:328:TYR:OH	2.16	0.45
2:C:315:GLY:HA2	2:C:320:SER:HB3	1.98	0.45
2:C:835:TYR:CZ	2:C:937:ARG:HD3	2.52	0.45
1:A:93:ARG:NH1	2:D:654:TYR:OH	2.48	0.45
2:D:698:SER:O	2:D:699:LEU:HD23	2.16	0.45
2:D:915:TRP:CD1	2:D:920:PRO:HA	2.51	0.45
1:B:23:GLU:N	1:B:23:GLU:OE1	2.37	0.45
2:D:280:LYS:HG2	2:D:281:TYR:CD1	2.51	0.45
1:A:36:TRP:NE1	1:A:129:LEU:HD22	2.31	0.45
1:A:275:ILE:HG22	1:A:284:LEU:CD1	2.46	0.45
1:A:263:ASN:HD21	1:A:401:ASN:HD22	1.65	0.45
2:C:703:SER:O	2:C:752:TYR:CD1	2.69	0.45
2:D:496:LEU:HA	2:D:496:LEU:HD12	1.66	0.45
2:D:722:MET:HE3	2:D:782:VAL:HG13	1.97	0.45
1:B:166:THR:O	1:B:170:GLN:N	2.45	0.45
2:D:585:LYS:HA	2:D:588:ARG:HG3	1.99	0.45
2:D:780:GLU:OE1	2:D:780:GLU:N	2.39	0.45
2:C:437:PRO:HG2	2:C:441:PHE:HE2	1.82	0.45
2:D:610:LEU:HD12	2:D:612:TRP:CZ2	2.51	0.45
2:D:616:LEU:HA	2:D:696:ASP:O	2.17	0.45
2:D:808:ILE:HG23	2:D:836:ARG:HG2	1.98	0.45
2:D:905:LEU:O	2:D:907:LYS:HD3	2.17	0.45
2:C:705:TYR:CZ	2:C:751:GLY:HA3	2.52	0.45
2:C:720:THR:HG21	2:C:788:PHE:HZ	1.82	0.45
2:D:262:ASN:O	2:D:274:TYR:HB2	2.17	0.45
1:A:389:CYS:HB2	1:A:399:SER:OG	2.17	0.44
2:C:950:LYS:NZ	2:C:996:GLU:HG2	2.32	0.44
1:A:4:PHE:CE1	2:D:553:SER:HB3	2.52	0.44
2:D:613:LEU:CD1	2:D:699:LEU:CD2	2.95	0.44
2:C:325:LEU:HA	2:C:325:LEU:HD23	1.80	0.44
2:D:424:TYR:HA	2:D:453:ASN:O	2.17	0.44
2:D:950:LYS:HD2	2:D:984:THR:CG2	2.46	0.44
1:B:62:GLY:O	1:B:369:SER:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:808:ILE:HG21	2:C:838:ILE:HD11	1.98	0.44
1:A:191:GLU:HG2	2:D:661:THR:HG22	1.99	0.44
2:D:643:TYR:HD2	2:D:671:SER:HB2	1.81	0.44
1:A:139:GLN:HB3	1:A:493:PHE:CD2	2.53	0.44
2:D:295:TRP:CZ3	2:D:410:PRO:HD2	2.53	0.44
2:D:400:PRO:HG2	2:D:468:GLN:HE21	1.82	0.44
2:C:641:PRO:HB3	2:C:673:PHE:CE1	2.52	0.44
1:A:54:ARG:HH21	1:A:493:PHE:HE1	1.64	0.44
1:B:478:LYS:HG2	1:B:498:TRP:CH2	2.52	0.44
2:D:807:TYR:O	2:D:939:SER:HA	2.17	0.44
2:C:888:SER:OG	2:C:889:ASP:N	2.49	0.44
1:A:277:ASP:HB2	2:D:669:LEU:HG	2.00	0.44
2:C:498:VAL:HG23	2:C:498:VAL:O	2.17	0.44
2:D:370:GLU:HB3	2:D:422:TYR:CZ	2.53	0.44
2:D:948:PHE:HA	2:D:985:ILE:O	2.17	0.44
1:A:148:ASN:OD1	1:A:148:ASN:N	2.51	0.44
1:A:19:ILE:HG13	2:D:639:TYR:CG	2.53	0.44
1:A:491:ARG:O	1:A:494:ASP:HB2	2.17	0.44
2:D:789:GLY:N	2:D:796:VAL:HG21	2.33	0.44
1:A:33:TYR:HB3	2:D:658:TYR:CD2	2.53	0.43
1:A:403:ILE:HG21	1:A:406:ARG:HG2	2.00	0.43
2:C:220:VAL:O	2:C:1009:THR:HG23	2.18	0.43
2:C:345:ARG:HG2	2:C:364:THR:HG23	2.00	0.43
2:C:695:ILE:O	2:C:707:SER:HA	2.18	0.43
2:C:313:SER:HB3	2:C:322:PHE:HD1	1.83	0.43
2:C:675:ARG:HD2	2:C:678:ILE:HG12	2.00	0.43
2:D:313:SER:HB3	2:D:322:PHE:HD1	1.83	0.43
2:D:569:TYR:OH	2:D:604:GLU:OE2	2.27	0.43
1:B:36:TRP:HE1	1:B:129:LEU:HD22	1.82	0.43
1:B:362:LYS:HA	1:B:375:TYR:CD1	2.54	0.43
1:B:51:TYR:CD1	1:B:532:LEU:HD11	2.53	0.43
1:B:11:GLN:HB2	2:C:549:GLY:O	2.18	0.43
2:D:523:LYS:HG2	2:D:539:GLY:HA3	2.00	0.43
2:D:748:PHE:HB3	2:D:768:ILE:HG23	2.01	0.43
1:A:138:LYS:HE3	1:A:171:TRP:CE2	2.52	0.43
2:C:352:LEU:HD12	2:C:357:LEU:CD1	2.47	0.43
2:C:577:ARG:HA	2:C:590:ALA:O	2.18	0.43
1:A:486:GLY:C	1:A:488:GLU:H	2.22	0.43
2:C:367:ARG:HG3	2:C:425:TRP:CE2	2.53	0.43
2:D:870:LYS:O	2:D:871:ASN:HB2	2.18	0.43
2:D:902:VAL:HG23	2:D:905:LEU:CD1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:VAL:HG22	1:B:107:SER:OG	2.18	0.43
2:C:370:GLU:HG2	2:C:371:VAL:N	2.34	0.43
1:B:100:ARG:NH2	2:C:674:LYS:HB2	2.34	0.43
2:C:751:GLY:HA2	2:C:764:LEU:O	2.19	0.43
2:C:807:TYR:O	2:C:939:SER:HA	2.18	0.43
2:C:872:PHE:CD2	2:C:956:LEU:HD21	2.53	0.43
2:D:427:MET:SD	2:D:427:MET:N	2.92	0.43
2:D:698:SER:C	2:D:699:LEU:HD23	2.39	0.43
2:C:966:LYS:HE3	2:C:966:LYS:HB3	1.82	0.43
2:C:370:GLU:HB3	2:C:422:TYR:CE2	2.54	0.43
2:C:568:ARG:CG	2:C:603:GLN:HB3	2.48	0.43
2:D:436:THR:HA	2:D:442:ASN:HB3	2.01	0.43
1:B:56:ASP:OD1	1:B:56:ASP:N	2.52	0.43
2:C:576:ARG:HD3	2:C:578:ASP:OD1	2.19	0.43
2:C:637:THR:HG22	2:C:679:GLY:H	1.84	0.43
2:D:242:TRP:O	2:D:246:VAL:HG13	2.19	0.43
1:A:222:LEU:HD13	1:A:499:GLY:HA3	2.01	0.42
1:A:42:ILE:HG21	1:A:395:TYR:CD2	2.54	0.42
1:A:474:MET:O	1:A:478:LYS:HG3	2.19	0.42
1:B:502:LYS:HG3	1:B:526:GLU:HB2	2.01	0.42
2:C:463:TYR:CD2	2:C:470:ASN:HB2	2.54	0.42
2:C:462:PRO:HD2	2:C:529:LEU:HD13	2.00	0.42
2:D:324:SER:HB3	2:D:345:ARG:HB2	2.01	0.42
2:D:915:TRP:HE1	2:D:920:PRO:HB3	1.84	0.42
1:B:142:LYS:HD2	1:B:531:TYR:CE2	2.54	0.42
1:B:127:ARG:NH2	1:B:177:ASP:OD1	2.49	0.42
2:C:426:ARG:NH1	2:C:450:ASP:OD2	2.52	0.42
2:C:563:TYR:CG	2:C:564:SER:N	2.87	0.42
2:C:712:TYR:OH	2:C:742:LYS:HE2	2.19	0.42
2:C:852:ILE:HD13	2:C:940:THR:HG22	2.00	0.42
2:D:365:LEU:HD12	2:D:366:ASN:N	2.34	0.42
2:D:857:PRO:HB3	2:D:884:VAL:HG22	1.99	0.42
2:C:221:SER:HA	2:C:1008:ILE:O	2.20	0.42
2:C:894:SER:O	2:C:911:LEU:HB3	2.19	0.42
2:D:318:LYS:O	2:D:351:LYS:N	2.45	0.42
2:D:560:LYS:HG3	2:D:574:THR:HG22	2.01	0.42
1:A:416:GLU:HB2	1:A:477:LEU:HD11	2.01	0.42
2:D:426:ARG:NH1	2:D:450:ASP:OD2	2.51	0.42
1:A:5:LEU:HD21	2:D:555:VAL:HG12	2.01	0.42
1:B:502:LYS:NZ	1:B:503:ASP:OD1	2.45	0.42
2:C:951:LEU:HD22	2:C:982:LEU:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:GLY:HA3	2:D:637:THR:OG1	2.20	0.42
2:D:950:LYS:HD2	2:D:984:THR:HG22	2.01	0.42
1:A:132:HIS:O	1:A:136:MET:HE2	2.20	0.42
2:D:586:ASN:HD22	2:D:587:HIS:CE1	2.38	0.42
1:B:412:LEU:HD23	1:B:412:LEU:HA	1.85	0.42
2:C:970:MET:HB3	2:C:971:ASP:H	1.40	0.42
2:D:278:LEU:HA	2:D:278:LEU:HD23	1.86	0.42
2:D:832:ARG:HB3	2:D:933:ASN:ND2	2.34	0.42
1:A:11:GLN:HB2	2:D:549:GLY:O	2.19	0.42
1:B:353:LYS:NZ	1:B:379:LEU:O	2.52	0.42
2:D:345:ARG:C	2:D:346:MET:HG3	2.40	0.42
2:D:362:HIS:O	2:D:429:GLY:HA3	2.20	0.42
2:D:950:LYS:HD3	2:D:984:THR:HB	2.02	0.42
1:A:320:PRO:HD3	1:A:437:ARG:NH2	2.34	0.42
2:D:535:TRP:HB3	2:C:547:GLY:O	2.20	0.42
2:C:805:VAL:HG12	2:C:849:GLN:HG3	2.02	0.42
2:D:234:THR:HG22	2:D:292:ASP:CG	2.40	0.42
2:D:443:LEU:H	2:D:443:LEU:HG	1.76	0.42
2:C:764:LEU:HD22	2:C:865:ILE:HG12	2.02	0.42
2:C:812:ILE:HG13	2:C:814:LYS:HE2	2.01	0.42
2:C:852:ILE:HD12	2:C:943:VAL:HG21	2.02	0.42
2:D:255:ASN:ND2	2:D:259:TYR:HB2	2.35	0.42
2:D:331:LEU:HA	2:D:331:LEU:HD23	1.69	0.42
2:D:643:TYR:CD2	2:D:671:SER:HB2	2.55	0.42
2:D:708:LEU:HD12	2:D:747:GLU:O	2.19	0.42
2:D:878:TRP:CE2	2:D:951:LEU:HD13	2.55	0.42
2:D:748:PHE:HB3	2:D:768:ILE:CG2	2.49	0.41
1:A:266:GLU:HG3	1:A:407:TYR:H	1.84	0.41
2:C:608:LYS:H	2:C:608:LYS:HG2	1.58	0.41
1:B:475:LYS:HB3	1:B:475:LYS:HE2	1.92	0.41
1:B:368:ARG:HG2	2:C:403:GLY:HA2	2.02	0.41
2:D:888:SER:HB2	2:D:998:PRO:HB2	2.01	0.41
2:C:377:ILE:HA	2:C:377:ILE:HD13	1.98	0.41
1:B:277:ASP:HB2	2:C:669:LEU:HG	2.01	0.41
2:C:236:GLN:O	2:C:239:ARG:N	2.53	0.41
2:C:258:GLY:CA	2:C:259:TYR:HB2	2.51	0.41
2:C:601:ILE:HG22	2:C:616:LEU:HB3	2.02	0.41
2:C:788:PHE:CD1	2:C:801:TYR:CE2	3.08	0.41
2:D:293:THR:HG21	2:D:295:TRP:CD2	2.56	0.41
1:A:475:LYS:HB3	1:A:475:LYS:HE2	1.90	0.41
1:B:426:ILE:O	1:B:430:ILE:HG12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:GLU:HB2	1:B:477:LEU:HD11	2.02	0.41
2:C:598:GLY:HA2	2:C:618:LEU:O	2.21	0.41
1:B:136:MET:HB2	1:B:136:MET:HE2	1.89	0.41
1:B:42:ILE:HG21	1:B:395:TYR:CD2	2.56	0.41
2:C:720:THR:HG21	2:C:788:PHE:CZ	2.55	0.41
2:C:244:ALA:HB2	2:C:927:LEU:HB3	2.03	0.41
2:D:498:VAL:O	2:D:501:HIS:HB2	2.20	0.41
2:D:789:GLY:CA	2:D:796:VAL:HG21	2.50	0.41
1:A:304:PRO:HG2	1:A:345:VAL:HG13	2.02	0.41
1:A:59:TYR:HA	1:A:75:GLU:OE2	2.21	0.41
2:C:808:ILE:HG21	2:C:808:ILE:HD13	1.77	0.41
2:C:986:LYS:N	2:C:986:LYS:HD2	2.19	0.41
2:D:528:ILE:HD12	2:D:533:TYR:CD1	2.56	0.41
2:D:699:LEU:N	2:D:704:LEU:O	2.49	0.41
2:D:694:GLY:HA2	2:D:709:GLU:HA	2.02	0.41
1:A:187:GLU:OE2	1:A:244:LYS:HD3	2.21	0.41
1:A:52:ASP:CG	1:A:489:SER:HA	2.41	0.41
1:B:155:ASP:OD1	1:B:155:ASP:N	2.38	0.41
2:C:616:LEU:HA	2:C:696:ASP:O	2.20	0.41
2:D:212:ILE:HD11	2:C:318:LYS:HB3	2.03	0.41
2:D:241:MET:HE1	2:D:255:ASN:HD22	1.85	0.41
2:D:414:LEU:HD23	2:D:414:LEU:HA	1.88	0.41
2:D:552:TYR:HE2	2:D:554:LEU:HD11	1.86	0.41
2:D:614:ASP:OD2	2:D:702:GLN:HG2	2.21	0.41
2:D:833:ILE:HD11	2:D:925:PRO:HG3	2.03	0.41
1:A:268:VAL:HB	1:A:405:ILE:O	2.21	0.41
2:C:334:ILE:HD11	2:C:378:ILE:HD11	2.03	0.41
2:C:338:ASP:O	2:C:370:GLU:HG3	2.21	0.41
2:D:233:ASN:HB2	2:D:236:GLN:CD	2.41	0.41
2:C:349:ASP:C	2:C:350:TYR:CD1	2.95	0.41
2:D:453:ASN:ND2	2:C:451:TYR:OH	2.54	0.41
2:D:866:TYR:O	2:D:867:LEU:HD12	2.21	0.41
1:A:400:LEU:HA	1:A:400:LEU:HD12	1.75	0.40
1:B:474:MET:HE3	1:B:478:LYS:HE3	2.03	0.40
2:C:704:LEU:HA	2:C:704:LEU:HD12	1.86	0.40
2:D:934:ASN:O	2:D:937:ARG:HD2	2.20	0.40
2:D:538:ALA:HA	2:C:641:PRO:HG2	2.03	0.40
2:D:588:ARG:HG2	2:D:588:ARG:HH11	1.86	0.40
1:A:283:ASN:ND2	2:D:657:ALA:O	2.53	0.40
1:B:463:TYR:CD1	1:B:476:MET:HE3	2.57	0.40
2:C:245:TYR:CD2	2:C:252:PRO:HA	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:891:LYS:HG2	2:C:895:ASP:OD2	2.20	0.40
2:C:232:LEU:N	2:C:906:ASN:HD21	2.06	0.40
2:C:909:THR:O	2:C:912:LEU:HB2	2.20	0.40
2:D:674:LYS:HG3	2:D:730:GLU:OE2	2.22	0.40
2:D:639:TYR:CZ	2:D:675:ARG:HB2	2.56	0.40
1:B:165:TYR:HB3	1:B:169:GLU:HB3	2.02	0.40
2:C:852:ILE:HB	2:C:940:THR:HG22	2.03	0.40
2:C:808:ILE:HA	2:C:940:THR:HG23	2.02	0.40
2:D:443:LEU:HA	2:D:492:ALA:HA	2.03	0.40
2:D:641:PRO:O	2:D:642:ASN:C	2.59	0.40
2:D:705:TYR:CE2	2:D:751:GLY:HA3	2.56	0.40
2:C:462:PRO:HD2	2:C:529:LEU:CD1	2.52	0.40
1:B:271:ILE:HA	2:C:658:TYR:OH	2.22	0.40
2:D:318:LYS:HD3	2:D:318:LYS:HA	1.50	0.40
2:D:382:LEU:HB3	2:D:893:LYS:NZ	2.37	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	552/576 (96%)	500 (91%)	48 (9%)	4 (1%)	26	65
1	B	553/576 (96%)	514 (93%)	36 (6%)	3 (0%)	34	72
2	C	805/1041 (77%)	716 (89%)	68 (8%)	21 (3%)	7	32
2	D	805/1041 (77%)	714 (89%)	72 (9%)	19 (2%)	7	33
All	All	2715/3234 (84%)	2444 (90%)	224 (8%)	47 (2%)	11	43

All (47) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	608	LYS
2	D	826	GLU
2	D	993	GLU
2	C	732	GLY
2	C	971	ASP
2	C	988	LYS
2	C	993	GLU
1	A	422	ASN
2	D	258	GLY
2	D	268	ASP
2	D	318	LYS
2	D	471	ASN
2	D	642	ASN
2	D	700	PHE
2	C	258	GLY
2	C	294	ASP
2	C	396	SER
2	C	406	ASP
2	C	826	GLU
2	C	970	MET
1	A	487	MET
1	A	491	ARG
2	D	375	GLY
2	D	845	ASP
1	B	267	SER
1	B	422	ASN
1	B	528	LYS
2	C	807	TYR
1	A	528	LYS
2	D	267	ALA
2	D	824	THR
2	D	971	ASP
2	C	437	PRO
2	C	797	VAL
2	C	822	HIS
2	D	396	SER
2	D	406	ASP
2	D	438	PHE
2	D	584	GLY
2	C	354	ASP
2	C	787	LYS
2	C	912	LEU
2	D	920	PRO

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Mol	Chain	Res	Type
2	C	718	ILE
2	C	1003	PRO
2	C	938	VAL
2	C	641	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	475/495 (96%)	469 (99%)	6 (1%)	76	91
1	B	476/495 (96%)	469 (98%)	7 (2%)	72	90
2	C	673/869 (77%)	644 (96%)	29 (4%)	35	72
2	D	673/869 (77%)	637 (95%)	36 (5%)	28	64
All	All	2297/2728 (84%)	2219 (97%)	78 (3%)	44	79

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASP
1	A	203	TYR
1	A	228	GLU
1	A	263	ASN
1	A	428	ASP
1	A	537	GLU
2	D	213	LYS
2	D	226	GLN
2	D	268	ASP
2	D	279	SER
2	D	317	GLU
2	D	341	ARG
2	D	354	ASP
2	D	357	LEU
2	D	470	ASN
2	D	502	ARG
2	D	506	MET

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Mol	Chain	Res	Type
2	D	516	ASP
2	D	517	SER
2	D	565	TYR
2	D	582	ARG
2	D	585	LYS
2	D	597	LEU
2	D	605	ASN
2	D	635	ARG
2	D	692	ASN
2	D	710	TYR
2	D	722	MET
2	D	730	GLU
2	D	747	GLU
2	D	753	ARG
2	D	754	ASN
2	D	772	ARG
2	D	773	ASN
2	D	787	LYS
2	D	801	TYR
2	D	834	ARG
2	D	895	ASP
2	D	910	ARG
2	D	911	LEU
2	D	950	LYS
2	D	971	ASP
1	B	3	ASP
1	B	17	ASP
1	B	106	GLN
1	B	203	TYR
1	B	228	GLU
1	B	317	GLN
1	B	502	LYS
2	C	228	LYS
2	C	278	LEU
2	C	426	ARG
2	C	427	MET
2	C	434	ASN
2	C	438	PHE
2	C	439	LYS
2	C	487	MET
2	C	504	ASP
2	C	506	MET

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Mol	Chain	Res	Type
2	C	565	TYR
2	C	568	ARG
2	C	569	TYR
2	C	586	ASN
2	C	597	LEU
2	C	614	ASP
2	C	628	GLN
2	C	684	LYS
2	C	696	ASP
2	C	701	LYS
2	C	747	GLU
2	C	814	LYS
2	C	834	ARG
2	C	969	ARG
2	C	970	MET
2	C	972	ARG
2	C	977	CYS
2	C	986	LYS
2	C	1012	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	ASN
2	D	255	ASN
2	D	849	GLN
1	B	106	GLN
1	B	110	GLN
2	C	442	ASN
2	C	791	ASN
2	C	906	ASN
2	C	913	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 5 ligands modelled in this entry, 5 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	552/576 (95%)	-0.38	1 (0%) 95 91	47, 83, 111, 146	0
1	B	553/576 (96%)	-0.33	0 100 100	37, 65, 95, 124	0
2	C	807/1041 (77%)	-0.43	0 100 100	37, 64, 104, 150	0
2	D	807/1041 (77%)	-0.39	0 100 100	35, 71, 111, 146	0
All	All	2719/3234 (84%)	-0.39	1 (0%) 100 100	35, 70, 108, 150	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	516	CYS	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 carbohydrates 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. 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	MG	C	1101	1/1	0.96	0.22	1.24	47,47,47,47	0
3	MG	A	601	1/1	0.97	0.16	-0.39	28,28,28,28	0
3	MG	B	602	1/1	0.94	0.17	-0.93	113,113,113,113	0
3	MG	A	602	1/1	0.83	0.09	-1.63	84,84,84,84	0
3	MG	B	601	1/1	0.96	0.12	-1.83	4,4,4,4	0

6.5 Other polymers [i](#)

There are no such residues in this entry.