



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:44 PM UTC

PDB ID : 5T4Y / pdb_00005t4y
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

<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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

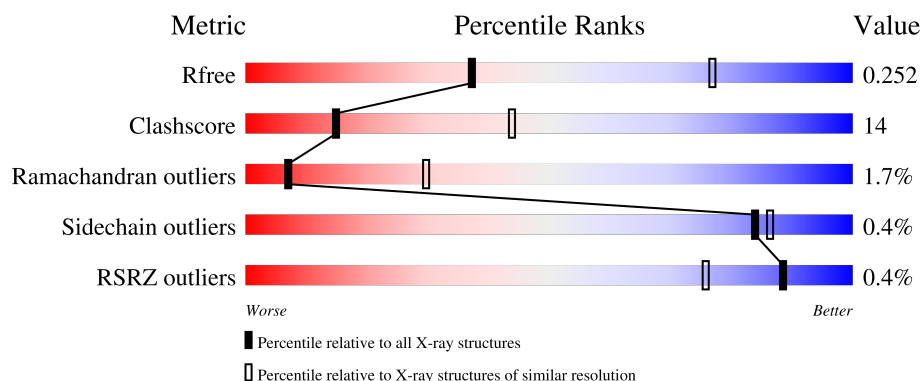
1 Overall quality at a glance

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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	576	76% 20% ••
1	B	576	% 75% 21% •
2	C	1041	49% 27% • 22%
2	D	1041	49% 27% • 22%

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			

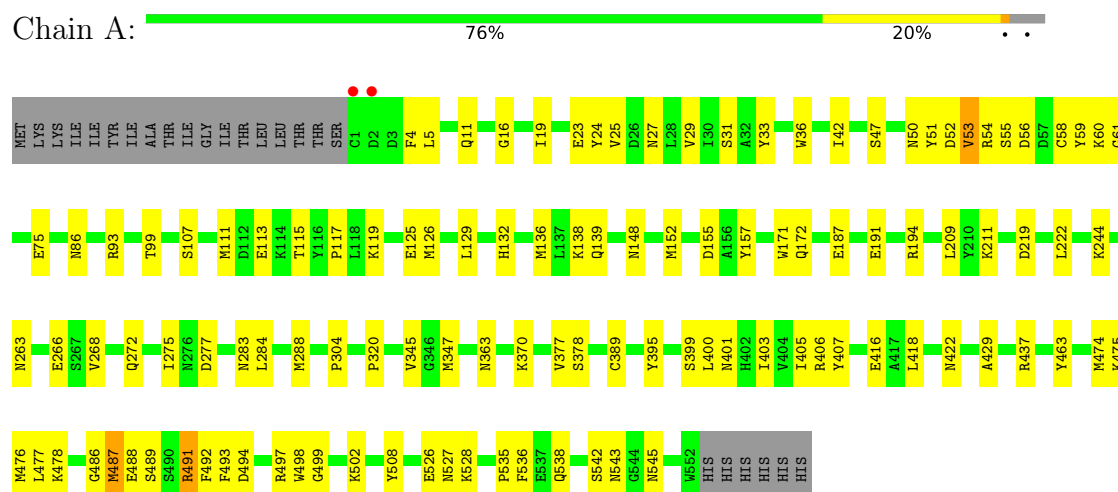
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

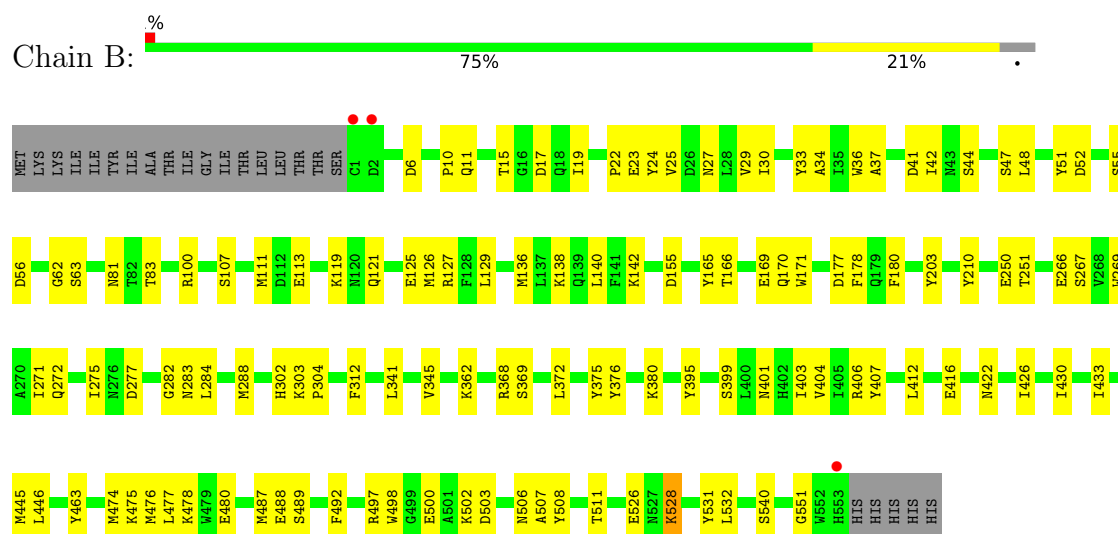
3 Residue-property plots

These plots are drawn for all protein, RNA, 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: SusD homolog



• Molecule 1: SusD homolog



• Molecule 2: SusC homolog



LEU	K318	G503	E604	G706	A823	P925
TYR	G319	D504	N605	S707	T824	A926
ILE	S320	V505	K608	L708	Q825	L927
ASP	S321	M506	K608	E709	E826	T928
GLY	K228	I507	W612	Y712	G827	N933
VAL	V231	G508	L616	L718	A828	K934
L232	N233	M509	L616	L718	R832	E935
PRO	T234	E510	L618	T720	Y835	Q936
THR	Q235	D516	L618	T720	R836	R937
LYS	Q236	D516	L618	T720	D837	V938
ALA	Y237	S520	Q624	G731	L838	S939
GLY	Y237	S520	Q624	G731	T940	T940
MET	G238	D525	Q628	G732	V943	V943
HIS	R239	D525	Q628	S733	D845	V943
GLU	Q243	I528	N632	R734	E846	V943
LEU	A244	L529	L633	R734	R847	K950
ASN	Y245	T530	L633	T736	Y735	L951
GLY	Y245	T530	L633	T736	L848	L951
ASN	V246	Y533	T637	G739	Q849	Q955
ASP	N247	A431	T638	K742	R850	L956
ILE	P252	Y432	Y639	F748	T852	S965
GLU	N255	V433	A640	F748	P641	K966
SER	Q258	N434	P641	G751	P857	K970
ILE	Y259	L435	N642	Y752	T865	D971
GLN	N262	T436	G541	L764	F872	R972
VAL	G258	I353	Y546	L768	D873	L973
LEU	Y259	D354	G547	L776	T875	R974
LYS	L272	D355	A548	E777	Y884	N981
ASP	Y274	I356	G549	K787	D885	L982
ALA	N263	L357	G549	F788	T886	K986
ALA	N266	G360	Y562	L776	L887	S987
SER	Y269	Q361	Y563	L776	S888	K988
ALA	V272	R362	S564	E777	D889	N989
SER	L273	F363	Y565	K787	V890	F990
ILE	Y274	T364	T456	F788	K891	T991
TYR	K280	R367	Y569	Y801	K893	G992
SER	Y281	E370	T574	Y801	S894	E993
ARG	L282	V371	L575	Q804	D895	E996
ALA	V290	P374	R576	V805	N901	K997
ASN	A291	G375	R577	G806	Y902	P998
GLY	D292	G376	D578	G807	G903	P1003
VAL	T293	I377	M470	T808	F904	V1006
ILE	D294	I378	N471	A809	L905	V1006
ILE	W295	E379	G472	D810	N906	V1007
THR	F296	T380	W483	T812	K907	T1009
THR	D297	D383	W487	F813	G908	T1009
LYS	E298	V390	N489	K814	T909	L1012
GLN	R301	S396	E487	T814	K910	L1013
LYS	V304	W397	V498	D817	L911	V1013
LYS	I305	P400	G499	E818	L912	L1014
G210	S313	V401	K500	H822	A914	G1015
G211	G315	G402	H501			F1016
I212			T602			
A218			Q603			
S219						

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 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.9 (130.35-3.10) 98.9 (130.35-3.10)	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 (Not available) , 0.252	Depositor DCC
R_{free} test set	4422 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	68.3	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 53.6	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

5.1 Standard geometry

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	0.38	0/4562	0.61	1/6190 (0.0%)
1	B	0.42	0/4573	0.68	0/6205
2	C	0.52	0/6571	0.78	5/8909 (0.1%)
2	D	0.48	0/6571	0.78	4/8909 (0.0%)
All	All	0.46	0/22277	0.73	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

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	470	ASN	N-CA-C	-8.99	100.15	114.09
2	C	565	TYR	CA-CB-CG	5.42	123.65	113.90
2	C	992	GLY	CA-C-N	5.34	131.75	121.54
2	C	992	GLY	C-N-CA	5.34	131.75	121.54
1	A	53	VAL	N-CA-C	-5.26	106.40	112.98
2	D	788	PHE	N-CA-C	5.07	119.52	113.23
2	D	258	GLY	CA-C-N	5.04	130.77	121.70
2	D	258	GLY	C-N-CA	5.04	130.77	121.70
2	C	987	SER	CA-C-N	5.01	131.11	121.54
2	C	987	SER	C-N-CA	5.01	131.11	121.54

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	90	0
1	B	4460	0	4227	89	0
2	C	6406	0	6058	217	0
2	D	6406	0	6058	231	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	585	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 14.

All (585) 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:HE3	2:C:427:MET:SD	1.39	1.58
2:D:427:MET:CE	2:C:427:MET:SD	2.35	1.12
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:H	2:C:986:LYS:HD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:832:ARG:NH1	2:D:935:GLU:OE2	2.17	0.77
2:C:568:ARG:NH2	2:C:603:GLN:O	2.18	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: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
1:A:25:VAL:HG22	1:A:107:SER:HB3	1.73	0.69
2:D:825:GLN:HG3	2:D:844:ILE:HG13	1.75	0.69
2:C:506:MET:HG2	2:C:507:ILE:N	2.08	0.69
1:A:5:LEU:HD12	2:D:588:ARG:HD3	1.74	0.68
1:A:272:GLN:OE1	1:A:401:ASN:ND2	2.22	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
2:D:607:MET:O	2:D:609:GLU:N	2.26	0.67
1:B:56:ASP:HA	1:B:508:TYR:CE2	2.30	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:383:ASP:HB3	2:C:893:LYS:HZ1	1.59	0.67
2:C:674:LYS:HE2	2:C:676:ASN:OD1	1.95	0.67
2:C:970:MET:HE2	2:C:973:LEU:HD22	1.77	0.66
1:B:416:GLU:CD	1:B:497:ARG:HH21	2.02	0.66
2:D:488:TRP:HZ3	2:D:509:MET:HE3	1.60	0.66
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:488:TRP:HZ3	2:C:509:MET:HE3	1.62	0.64
1:A:58:CYS:HB3	1:A:487:MET:HE1	1.80	0.64
2:D:760:LEU:HD12	2:D:869:TYR:HB2	1.77	0.64
2:D:902:VAL:HG23	2:D:905:LEU:HD11	1.78	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:C:528:ILE:HG22	2:C:530:THR:HG22	1.79	0.64
2:D:722:MET:HE3	2:D:782:VAL:HG13	1.79	0.64
2:C:374:PRO:HD2	2:C:377:ILE:HG13	1.78	0.64
2:C:488:TRP:CZ3	2:C:509:MET:HE3	2.33	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:D:334:ILE:HD11	2:D:378:ILE:HD11	1.80	0.63
2:C:987:SER:O	2:C:989:ASN:N	2.31	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:241:MET:HE3	2:D:255:ASN:HD22	1.65	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
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:24:TYR:O	1:A:27:ASN:HB2	2.01	0.61
1:A:138:LYS:HG2	1:A:171:TRP:CH2	2.36	0.61
2:C:301:ARG:HG3	2:C:335:LYS:HG2	1.82	0.60
1:A:29:VAL:HG13	1:A:126:MET:HE3	1.83	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
2:D:370:GLU:HB3	2:D:422:TYR:CE2	2.37	0.59
2:C:682:ASN:ND2	2:C:682:ASN:O	2.35	0.59
2:D:279:SER:O	2:D:281:TYR:N	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:682:ASN:O	2:D:682:ASN:ND2	2.36	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: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
2:D:637:THR:HG23	2:D:679:GLY:H	1.68	0.58
1:B:416:GLU:OE1	1:B:497:ARG:NH2	2.36	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:345:ARG:C	2:C:346:MET:HG3	2.30	0.56
2:C:648:SER:HB3	2:C:651:GLY:O	2.05	0.56
2:C:825:GLN:HB3	2:C:828:ALA:HB2	1.87	0.56
2:D:780:GLU:H	2:D:780:GLU:CD	2.13	0.56
2:D:587:HIS:CD2	2:D:684:LYS:HB3	2.41	0.56
1:B:34:ALA:O	1:B:37:ALA:N	2.39	0.56
2:C:487:MET:HE2	2:C:510:GLU:OE1	2.05	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:D:336:ASP:OD2	2:D:411:ARG:NH2	2.39	0.55
2:C:748:PHE:HB3	2:C:768:ILE:HG23	1.88	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: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
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
1:B:6:ASP:OD2	2:C:588:ARG:NH2	2.39	0.55
1:B:275:ILE:HG23	1:B:399:SER:HB3	1.89	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
2:D:835:TYR:CE1	2:D:937:ARG:HD3	2.42	0.54
1:B:138:LYS:HG2	1:B:171:TRP:CZ2	2.41	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:D:808:ILE:HA	2:D:940:THR:HG23	1.90	0.54
2:C:914:ALA:HB1	2:C:925:PRO:O	2.08	0.54
1:A:474:MET:HE3	1:A:478:LYS:HE3	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:D:574:THR:OG1	2:D:594:SER:HB3	2.08	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
1:A:31:SER:HB2	2:D:672:GLY:HA3	1.90	0.53
2:D:791:ASN:HD21	2:D:804:GLN:HG2	1.74	0.53
2:C:353:ILE:HG22	2:C:356:ILE:HB	1.90	0.53
2:D:993:GLU:OE2	2:D:993:GLU:HA	2.09	0.53
2:C:228:LYS:HD3	2:C:296:PHE:CG	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:585:LYS:HA	2:C:588:ARG:HG3	1.89	0.53
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:234:THR:HG22	2:C:292:ASP:CG	2.34	0.53
2:C:605:ASN:HA	2:C:608:LYS:CE	2.39	0.53
1:A:23:GLU:OE1	1:A:23:GLU:N	2.24	0.52
2:C:951:LEU:HD23	2:C:951:LEU:O	2.09	0.52
2:D:652:GLN:HB3	2:D:654:TYR:HE1	1.75	0.52
1:B:121:GLN:O	1:B:125:GLU:HG3	2.09	0.52
1:B:10:PRO:HB3	2:C:633:LEU:HD23	1.91	0.52
1:B:52:ASP:CG	1:B:489:SER:HA	2.35	0.52
2:C:263:TRP:H	2:C:263:TRP:CD1	2.26	0.52
2:D:807:TYR:CD2	2:D:937:ARG:HG3	2.45	0.52
2:C:360:GLY:HA3	2:C:432:TYR:CZ	2.45	0.52
2:D:415:GLU:O	2:D:418:LYS:HG2	2.09	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
1:B:302:HIS:CE1	1:B:487:MET:HE3	2.45	0.52
2:C:906:ASN:C	2:C:907:LYS:HD2	2.35	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: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
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:A:370:LYS:HG3	2:D:256:ALA:HA	1.91	0.52
1:B:29:VAL:HG13	1:B:126:MET:HE3	1.90	0.52
1:B:36:TRP:NE1	1:B:129:LEU:HD22	2.25	0.52
2:D:232:LEU:HD22	2:D:907:LYS:O	2.09	0.51
2:D:241:MET:CE	2:D:255:ASN:HD22	2.24	0.51
2:C:578:ASP:O	2:C:589:TYR:HA	2.11	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:D:528:ILE:HB	2:D:533:TYR:CG	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:718:ILE:O	2:D:737:ASN:HA	2.10	0.50
2:C:401:VAL:HA	2:C:467:THR:HG23	1.92	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:36:TRP:HZ3	1:B:136:MET:HE1	1.76	0.50
1:B:403:ILE:HG21	1:B:406:ARG:HG2	1.92	0.50
2:D:279:SER:O	2:D:279:SER:OG	2.21	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
2:C:901:ASN:O	2:C:901:ASN:ND2	2.45	0.50
2:D:854:ASP:O	2:D:885:ASP:HB2	2.12	0.50
1:B:177:ASP:O	1:B:180:PHE:N	2.43	0.50
1:A:155:ASP:OD1	1:A:155:ASP:N	2.45	0.50
2:D:255:ASN:HD21	2:D:258:GLY:HA2	1.77	0.50
1:B:15:THR:C	1:B:17:ASP:H	2.20	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: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:574:THR:OG1	2:C:594:SER:HB3	2.12	0.50
2:D:652:GLN:HB3	2:D:654:TYR:CE1	2.47	0.49
1:B:540:SER:OG	2:C:792:GLY:O	2.30	0.49
2:C:568:ARG:HD2	2:C:569:TYR:CE2	2.47	0.49
2:C:808:ILE:HG23	2:C:836:ARG:HG2	1.94	0.49
1:A:152:MET:HB3	1:A:157:TYR:HE2	1.76	0.49
2:D:547:GLY:O	2:C:535:TRP:HB3	2.11	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:805:VAL:HG12	2:D:849:GLN:HG3	1.95	0.49
2:D:824:THR:OG1	2:D:843:VAL:HG12	2.12	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
1:B:41:ASP:HB3	1:B:44:SER:OG	2.13	0.49
1:A:47:SER:CB	1:A:288:MET:HE1	2.42	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:36:TRP:CZ3	1:B:136:MET:HE1	2.47	0.49
2:C:647:ASP:OD1	2:C:648:SER:N	2.45	0.49
1:B:507:ALA:O	1:B:511:THR:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:362:HIS:O	2:C:429:GLY:HA3	2.13	0.49
2:D:788:PHE:N	2:D:789:GLY:HA3	2.27	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: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
1:B:47:SER:CB	1:B:288:MET:HE1	2.43	0.49
1:B:474:MET:HE3	1:B:478:LYS:HE3	1.95	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
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: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:905:LEU:HB2	2:C:907:LYS:HE2	1.94	0.48
2:D:965:SER:O	2:D:970:MET:HB2	2.14	0.48
1:A:486:GLY:C	1:A:488:GLU:H	2.22	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
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: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
2:D:698:SER:C	2:D:699:LEU:HD23	2.39	0.48
1:B:283:ASN:ND2	2:C:657:ALA:O	2.45	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
2:C:734:ARG:HG3	2:C:736:ILE:HG23	1.95	0.48
1:A:363:ASN:OD1	1:A:363:ASN:N	2.47	0.47
2:D:953:ASN:ND2	2:D:979:ALA:O	2.38	0.47
2:C:637:THR:CG2	2:C:679:GLY:H	2.26	0.47
1:A:99:THR:OG1	2:D:729:GLY:HA3	2.14	0.47
2:D:397:TRP:HZ2	2:D:415:GLU:HG3	1.79	0.47
2:D:902:VAL:CG2	2:D:905:LEU:HD11	2.43	0.47
1:A:463:TYR:CG	1:A:476:MET:HE3	2.50	0.47
2:C:252:PRO:O	2:C:255:ASN:ND2	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:30:ILE:HG13	2:C:660:ILE:HG13	1.97	0.47
1:B:463:TYR:CD1	1:B:476:MET:HE3	2.49	0.47
2:C:791:ASN:HD21	2:C:804:GLN:HG2	1.79	0.47
1:A:463:TYR:CD1	1:A:476:MET:HE3	2.50	0.47
2:D:364:THR:HB	2:D:428:PHE:CE1	2.50	0.47
2:D:383:ASP:HB2	2:D:905:LEU:HB3	1.97	0.47
1:B:19:ILE:HG13	2:C:639:TYR:CD2	2.50	0.47
2:D:462:PRO:HB3	2:D:472:GLY:HA2	1.97	0.47
2:D:242:TRP:HE1	2:D:263:TRP:CG	2.33	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:612:TRP:H	2:C:612:TRP:CD1	2.32	0.47
2:C:857:PRO:HA	2:C:884:VAL:HG12	1.97	0.47
2:D:345:ARG:C	2:D:346:MET:HG3	2.40	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
2:D:234:THR:HG22	2:D:292:ASP:CG	2.40	0.46
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:132:HIS:CE1	1:A:136:MET:HE2	2.50	0.46
1:A:263:ASN:HD21	1:A:401:ASN:ND2	2.14	0.46
2:D:878:TRP:CZ3	2:D:951:LEU:HB2	2.50	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
1:A:56:ASP:HA	1:A:508:TYR:CE2	2.50	0.46
1:A:209:LEU:HD21	1:A:497:ARG:NE	2.29	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: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:C:408:ARG:HG3	2:C:468:GLN:HG2	1.97	0.46
2:C:422:TYR:HA	2:C:456:ALA:HB2	1.95	0.46
1:B:502:LYS:O	1:B:506:ASN:ND2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:970:MET:HE3	2:C:1014:ILE:HD13	1.98	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: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
1:A:275:ILE:HG21	1:A:275:ILE:HD13	1.69	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
2:C:530:THR:HG23	2:C:533:TYR:H	1.80	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
1:A:52:ASP:CG	1:A:489:SER:HA	2.41	0.45
2:D:276:MET:HE3	2:D:276:MET:HB2	1.77	0.45
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
2:C:349:ASP:C	2:C:350:TYR:CD1	2.95	0.45
1:A:486:GLY:O	1:A:488:GLU:N	2.50	0.45
2:D:233:ASN:HB2	2:D:236:GLN:CD	2.41	0.45
2:C:822:HIS:CG	2:C:823:ALA:H	2.33	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
2:C:400:PRO:O	2:C:466:GLY:HA3	2.17	0.45
1:A:93:ARG:NH1	2:D:654:TYR:OH	2.48	0.45
2:D:488:TRP:CZ3	2:D:509:MET:HE3	2.46	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: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
2:D:280:LYS:HG2	2:D:281:TYR:CD1	2.51	0.45
1:B:23:GLU:OE1	1:B:23:GLU:N	2.37	0.45
1:A:36:TRP:NE1	1:A:129:LEU:HD22	2.31	0.45
1:A:263:ASN:HD21	1:A:401:ASN:HD22	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ILE:HG22	1:A:284:LEU:CD1	2.46	0.45
2:D:496:LEU:HD12	2:D:496:LEU:HA	1.66	0.45
2:D:641:PRO:O	2:D:642:ASN:C	2.59	0.45
2:C:703:SER:O	2:C:752:TYR:CD1	2.69	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
1:B:166:THR:O	1:B:170:GLN:N	2.45	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:437:PRO:HG2	2:C:441:PHE:HE2	1.82	0.45
2:C:489:ASN:OD1	2:C:489:ASN:C	2.59	0.45
2:D:262:ASN:O	2:D:274:TYR:HB2	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
1:A:4:PHE:CE1	2:D:553:SER:HB3	2.52	0.44
1:A:389:CYS:HB2	1:A:399:SER:OG	2.17	0.44
2:D:613:LEU:CD1	2:D:699:LEU:CD2	2.95	0.44
2:C:950:LYS:NZ	2:C:996:GLU:HG2	2.32	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
2:C:325:LEU:HD23	2:C:325:LEU:HA	1.80	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:B:62:GLY:O	1:B:369:SER:HB3	2.17	0.44
2:C:808:ILE:HG21	2:C:838:ILE:HD11	1.98	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
2:D:807:TYR:O	2:D:939:SER:HA	2.17	0.44
1:B:478:LYS:HG2	1:B:498:TRP:CH2	2.52	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:D:370:GLU:HB3	2:D:422:TYR:CZ	2.53	0.44
2:D:839:ASP:HB3	2:D:841:ASN:CG	2.42	0.44
2:D:948:PHE:HA	2:D:985:ILE:O	2.17	0.44
2:C:498:VAL:HG23	2:C:498:VAL:O	2.17	0.44
1:A:19:ILE:HG13	2:D:639:TYR:CG	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ASN:OD1	1:A:148:ASN:N	2.51	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:B:47:SER:HB3	1:B:288:MET:HE1	1.99	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: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
2:D:576:ARG:HH11	2:D:578:ASP:CG	2.26	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
1:B:36:TRP:HE1	1:B:129:LEU:HD22	1.82	0.43
1:B:51:TYR:CD1	1:B:532:LEU:HD11	2.53	0.43
1:B:362:LYS:HA	1:B:375:TYR:CD1	2.54	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:B:11:GLN:HB2	2:C:549:GLY:O	2.18	0.43
1:A:111:MET:HE3	1:A:111:MET:HA	1.99	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
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
2:C:367:ARG:HG3	2:C:425:TRP:CE2	2.53	0.43
2:D:427:MET:SD	2:D:427:MET:N	2.92	0.43
1:B:25:VAL:HG22	1:B:107:SER:OG	2.18	0.43
1:B:100:ARG:NH2	2:C:674:LYS:HB2	2.34	0.43
2:C:370:GLU:HG2	2:C:371:VAL:N	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:344:ALA:HB1	2:D:346:MET:HE3	2.01	0.43
2:C:966:LYS:HE3	2:C:966:LYS:HB3	1.82	0.43
2:D:436:THR:HA	2:D:442:ASN:HB3	2.01	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:242:TRP:O	2:D:246:VAL:HG13	2.19	0.43
1:B:56:ASP:OD1	1:B:56:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:42:ILE:HG21	1:A:395:TYR:CD2	2.54	0.42
1:A:222:LEU:HD13	1:A:499:GLY:HA3	2.01	0.42
1:A:474:MET:O	1:A:478:LYS:HG3	2.19	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:502:LYS:HG3	1:B:526:GLU:HB2	2.01	0.42
2:C:462:PRO:HD2	2:C:529:LEU:HD13	2.00	0.42
2:C:463:TYR:CD2	2:C:470:ASN:HB2	2.54	0.42
1:A:219:ASP:HB2	1:A:527:ASN:CG	2.44	0.42
2:D:365:LEU:HD12	2:D:366:ASN:N	2.34	0.42
2:D:786:GLY:C	2:D:789:GLY:HA3	2.44	0.42
2:D:857:PRO:HB3	2:D:884:VAL:HG22	1.99	0.42
1:B:81:ASN:C	1:B:83:THR:H	2.27	0.42
1:B:127:ARG:NH2	1:B:177:ASP:OD1	2.49	0.42
1:B:142:LYS:HD2	1:B:531:TYR:CE2	2.54	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:318:LYS:O	2:D:351:LYS:N	2.45	0.42
2:D:536:PRO:HB2	2:C:546:TYR:C	2.44	0.42
2:D:560:LYS:HG3	2:D:574:THR:HG22	2.01	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
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: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: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
1:A:47:SER:OG	1:A:288:MET:HE1	2.19	0.42
2:D:586:ASN:HD22	2:D:587:HIS:CE1	2.38	0.42
2:D:278:LEU:HD23	2:D:278:LEU:HA	1.86	0.42
2:D:832:ARG:HB3	2:D:933:ASN:ND2	2.34	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
1:A:11:GLN:HB2	2:D:549:GLY:O	2.19	0.42
2:D:362:HIS:O	2:D:429:GLY:HA3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:950:LYS:HD3	2:D:984:THR:HB	2.02	0.42
1:B:47:SER:OG	1:B:288:MET:HE1	2.20	0.42
1:A:320:PRO:HD3	1:A:437:ARG:NH2	2.34	0.42
2:D:443:LEU:H	2:D:443:LEU:HG	1.76	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:C:806:GLY:C	2:C:849:GLN:HB2	2.44	0.42
2:D:255:ASN:ND2	2:D:259:TYR:HB2	2.35	0.42
2:D:331:LEU:HD23	2:D:331:LEU:HA	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
1:B:463:TYR:CG	1:B:476:MET:HE3	2.55	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:748:PHE:HB3	2:D:768:ILE:CG2	2.49	0.41
1:B:177:ASP:O	1:B:178:PHE:C	2.62	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
2:D:888:SER:HB2	2:D:998:PRO:HB2	2.01	0.41
1:B:368:ARG:HG2	2:C:403:GLY:HA2	2.02	0.41
1:B:475:LYS:HE2	1:B:475:LYS:HB3	1.92	0.41
1:B:277:ASP:HB2	2:C:669:LEU:HG	2.01	0.41
2:C:377:ILE:HD13	2:C:377:ILE:HA	1.98	0.41
2:D:293:THR:HG21	2:D:295:TRP:CD2	2.56	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
1:A:475:LYS:HB3	1:A:475:LYS:HE2	1.90	0.41
1:B:416:GLU:HB2	1:B:477:LEU:HD11	2.02	0.41
1:B:426:ILE:O	1:B:430:ILE:HG12	2.21	0.41
2:C:598:GLY:HA2	2:C:618:LEU:O	2.21	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:B:42:ILE:HG21	1:B:395:TYR:CD2	2.56	0.41
2:C:244:ALA:HB2	2:C:927:LEU:HB3	2.03	0.41
2:C:720:THR:HG21	2:C:788:PHE:CZ	2.55	0.41
1:A:59:TYR:HA	1:A:75:GLU:OE2	2.21	0.41
1:A:304:PRO:HG2	1:A:345:VAL:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:528:ILE:HD12	2:D:533:TYR:CD1	2.56	0.41
2:D:694:GLY:HA2	2:D:709:GLU:HA	2.02	0.41
2:D:699:LEU:N	2:D:704:LEU:O	2.49	0.41
2:C:808:ILE:HG21	2:C:808:ILE:HD13	1.77	0.41
2:C:986:LYS:HD2	2:C:986:LYS:N	2.19	0.41
1:A:187:GLU:OE2	1:A:244:LYS:HD3	2.21	0.41
1:A:268:VAL:HB	1:A:405:ILE:O	2.21	0.41
1:A:347:MET:HE3	1:A:347:MET:HB2	1.84	0.41
2:D:212:ILE:HD11	2:C:318:LYS:HB3	2.03	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:B:155:ASP:OD1	1:B:155:ASP:N	2.38	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:C:616:LEU:HA	2:C:696:ASP:O	2.20	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
2:D:805:VAL:HG13	2:D:850:ASN:C	2.46	0.40
2:D:934:ASN:O	2:D:937:ARG:HD2	2.20	0.40
2:C:704:LEU:HD12	2:C:704:LEU:HA	1.86	0.40
1:A:283:ASN:ND2	2:D:657:ALA:O	2.53	0.40
2:D:538:ALA:HA	2:C:641:PRO:HG2	2.03	0.40
2:D:588:ARG:HH11	2:D:588:ARG:HG2	1.86	0.40
2:D:639:TYR:CZ	2:D:675:ARG:HB2	2.56	0.40
2:D:674:LYS:HG3	2:D:730:GLU:OE2	2.22	0.40
2:C:232:LEU:N	2:C:906:ASN:HD21	2.06	0.40
2:C:245:TYR:CD2	2:C:252:PRO:HA	2.57	0.40
2:C:891:LYS:HG2	2:C:895:ASP:OD2	2.20	0.40
2:C:909:THR:O	2:C:912:LEU:HB2	2.20	0.40
2:D:443:LEU:HA	2:D:492:ALA:HA	2.03	0.40
2:D:705:TYR:CE2	2:D:751:GLY:HA3	2.56	0.40
1:B:165:TYR:HB3	1:B:169:GLU:HB3	2.02	0.40
2:C:808:ILE:HA	2:C:940:THR:HG23	2.02	0.40
2:C:852:ILE:HB	2:C:940:THR:HG22	2.03	0.40
2:D:318:LYS:HA	2:D:318:LYS:HD3	1.50	0.40
2:D:382:LEU:HB3	2:D:893:LYS:NZ	2.37	0.40
1:B:271:ILE:HA	2:C:658:TYR:OH	2.22	0.40
2:C:462:PRO:HD2	2:C:529:LEU:CD1	2.52	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%)	18	49
1	B	553/576 (96%)	514 (93%)	36 (6%)	3 (0%)	24	57
2	C	805/1041 (77%)	716 (89%)	68 (8%)	21 (3%)	4	21
2	D	805/1041 (77%)	714 (89%)	72 (9%)	19 (2%)	4	22
All	All	2715/3234 (84%)	2444 (90%)	224 (8%)	47 (2%)	7	30

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

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Mol	Chain	Res	Type
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
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%)	475 (100%)	0	100	100
1	B	476/495 (96%)	474 (100%)	2 (0%)	84	86
2	C	673/869 (77%)	668 (99%)	5 (1%)	76	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	673/869 (77%)	670 (100%)	3 (0%)	84	86
All	All	2297/2728 (84%)	2287 (100%)	10 (0%)	84	86

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	516	ASP
2	D	709	GLU
2	D	971	ASP
1	B	203	TYR
1	B	251	THR
2	C	357	LEU
2	C	380	THR
2	C	504	ASP
2	C	564	SER
2	C	709	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	ASN
1	A	302	HIS
1	A	457	ASN
2	D	255	ASN
2	D	468	GLN
2	D	544	GLN
2	D	677	GLN
2	D	743	ASN
2	D	849	GLN
1	B	18	GLN
1	B	27	ASN
1	B	88	ASN
1	B	106	GLN
1	B	110	GLN
1	B	170	GLN
1	B	276	ASN
2	C	262	ASN
2	C	330	ASN
2	C	442	ASN
2	C	692	ASN
2	C	743	ASN

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Mol	Chain	Res	Type
2	C	791	ASN
2	C	821	ASN
2	C	871	ASN
2	C	882	GLN
2	C	901	ASN
2	C	906	ASN
2	C	934	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	2 (0%)	88 76	44, 83, 111, 146	2 (0%)
1	B	553/576 (96%)	-0.56	3 (0%)	87 73	37, 65, 94, 124	2 (0%)
2	C	807/1041 (77%)	-0.37	2 (0%)	91 83	37, 64, 104, 150	0
2	D	807/1041 (77%)	-0.30	5 (0%)	85 70	35, 71, 111, 146	0
All	All	2719/3234 (84%)	-0.39	12 (0%)	88 76	35, 70, 108, 150	4 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	553	HIS	4.4
1	A	1	CYS	3.5
1	B	1	CYS	3.0
1	B	2	ASP	2.7
2	D	427	MET	2.5
1	A	2	ASP	2.5
2	D	210	GLY	2.5
2	D	858	SER	2.4
2	D	909	THR	2.4
2	C	986	LYS	2.3
2	C	848	ASP	2.3
2	D	848	ASP	2.1

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	MG	B	602	1/1	0.92	0.12	113,113,113,113	0
3	MG	A	602	1/1	0.97	0.05	84,84,84,84	0
3	MG	C	1101	1/1	0.98	0.11	47,47,47,47	0
3	MG	A	601	1/1	0.99	0.03	28,28,28,28	0
3	MG	B	601	1/1	1.00	0.05	4,4,4,4	0

6.5 Other polymers [i](#)

There are no such residues in this entry.