



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:05 AM UTC

PDB ID : 3BGA / pdb_00003bga
Title : Crystal structure of beta-galactosidase from Bacteroides thetaiotaomicron VPI-5482
Authors : Kumaran, D.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2007-11-26
Resolution : 2.10 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

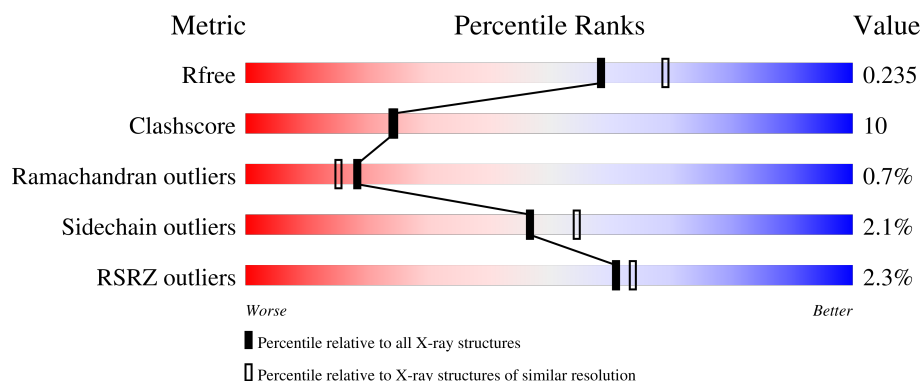
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	1010	2% 77% 20% ...
1	B	1010	2% 76% 21% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17243 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 Beta-galactosidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1003	Total	C	N	O	S	Se	0	0	0
			8064	5124	1390	1516	14	20			
1	B	1000	Total	C	N	O	S	Se	0	0	0
			8034	5109	1379	1512	14	20			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MSE	-	expression tag	UNP Q8A799
A	22	SER	-	expression tag	UNP Q8A799
A	23	LEU	-	expression tag	UNP Q8A799
A	1023	GLU	-	expression tag	UNP Q8A799
A	1024	GLY	-	expression tag	UNP Q8A799
A	1025	HIS	-	expression tag	UNP Q8A799
A	1026	HIS	-	expression tag	UNP Q8A799
A	1027	HIS	-	expression tag	UNP Q8A799
A	1028	HIS	-	expression tag	UNP Q8A799
A	1029	HIS	-	expression tag	UNP Q8A799
A	1030	HIS	-	expression tag	UNP Q8A799
B	21	MSE	-	expression tag	UNP Q8A799
B	22	SER	-	expression tag	UNP Q8A799
B	23	LEU	-	expression tag	UNP Q8A799
B	1023	GLU	-	expression tag	UNP Q8A799
B	1024	GLY	-	expression tag	UNP Q8A799
B	1025	HIS	-	expression tag	UNP Q8A799
B	1026	HIS	-	expression tag	UNP Q8A799
B	1027	HIS	-	expression tag	UNP Q8A799
B	1028	HIS	-	expression tag	UNP Q8A799
B	1029	HIS	-	expression tag	UNP Q8A799
B	1030	HIS	-	expression tag	UNP Q8A799

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Na 2 2	0	0
3	B	2	Total Na 2 2	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0

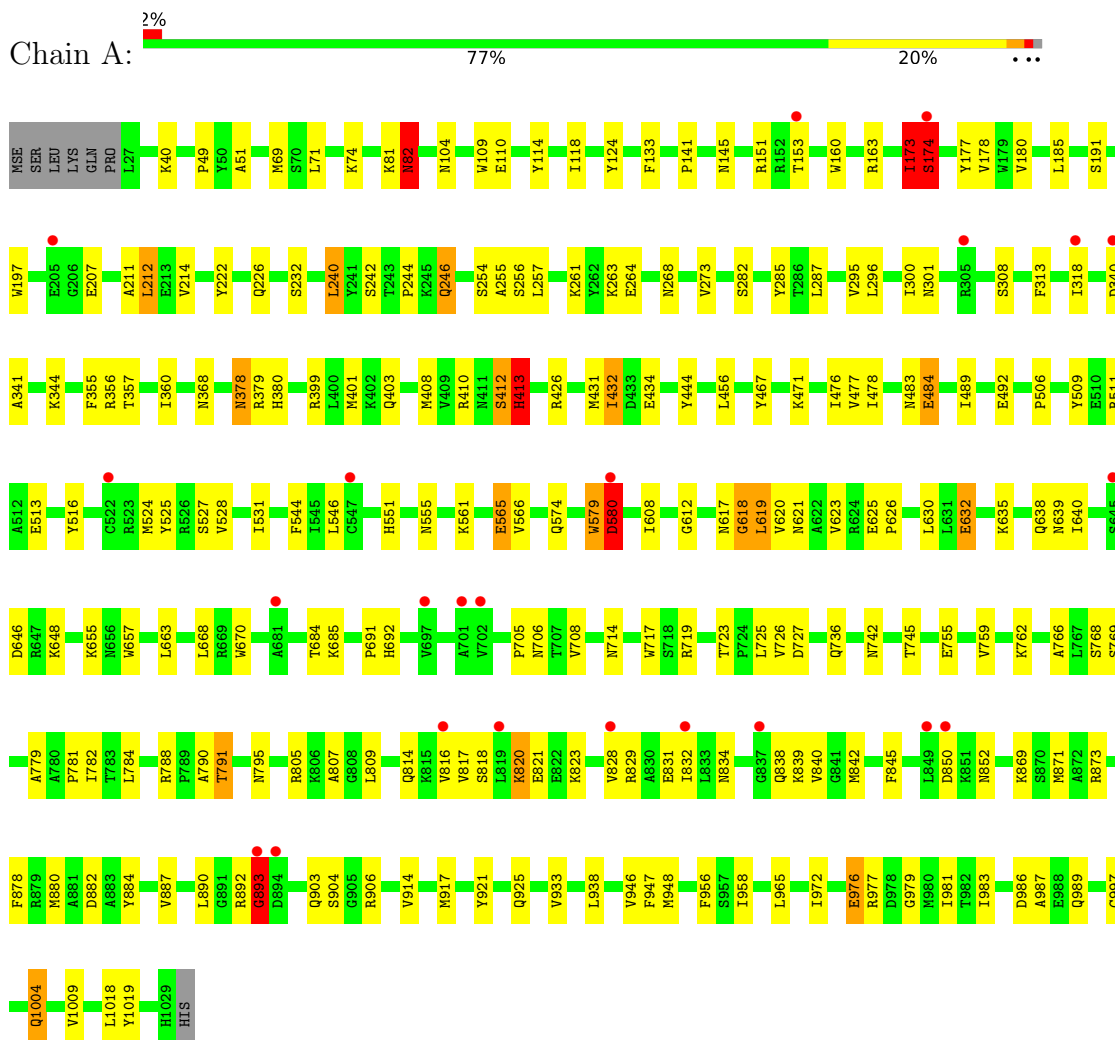
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	563	Total O 563 563	0	0
5	B	574	Total O 574 574	0	0

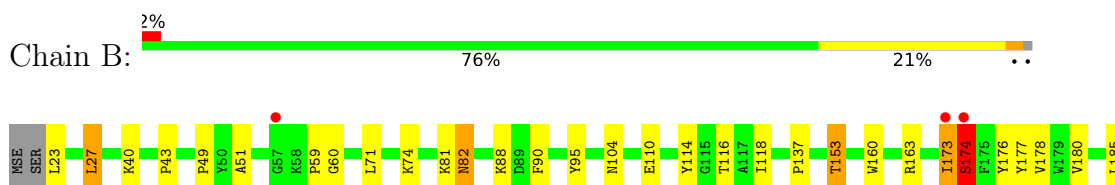
3 Residue-property plots [i](#)

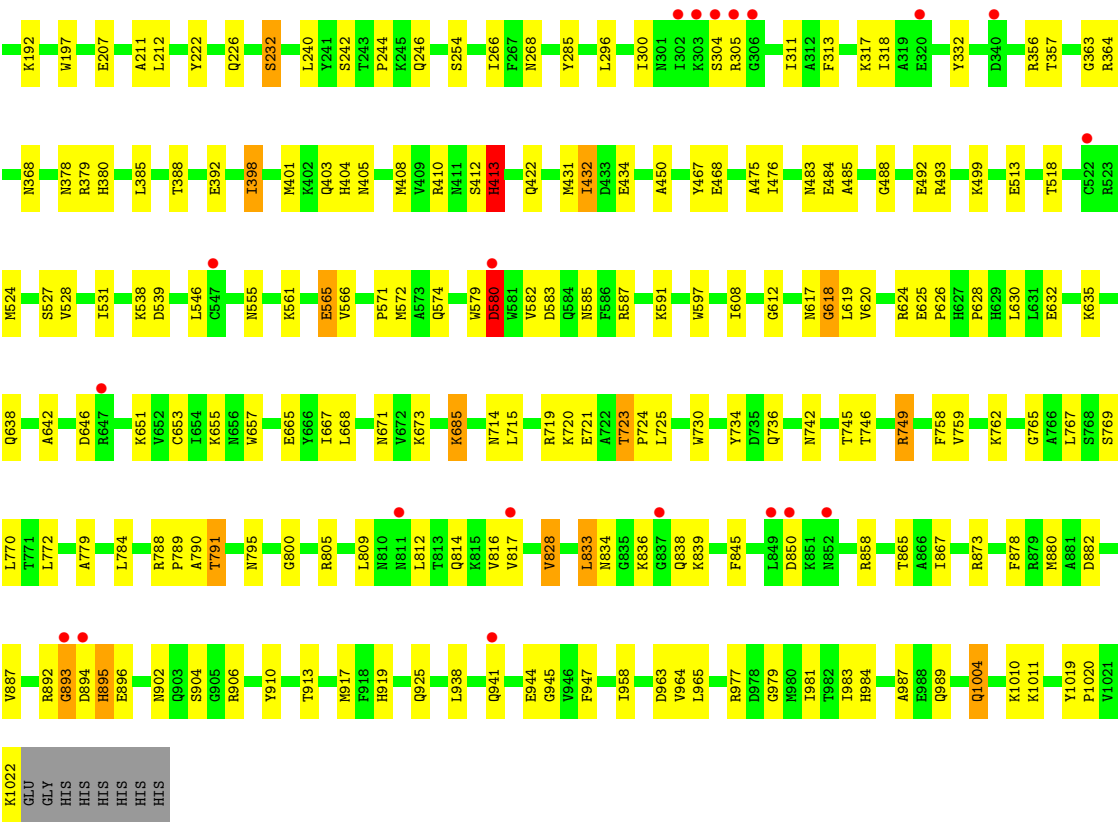
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Beta-galactosidase



• Molecule 1: Beta-galactosidase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.33Å 138.86Å 102.82Å 90.00° 109.73° 90.00°	Depositor
Resolution (Å)	49.76 – 2.10 49.76 – 2.10	Depositor EDS
% Data completeness (in resolution range)	84.7 (49.76-2.10) 84.8 (49.76-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.50 (at 2.08Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.200 , 0.234 0.200 , 0.235	Depositor DCC
R_{free} test set	5795 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.737	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.1	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	0.93	EDS
Total number of atoms	17243	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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: NA, MG, CL

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	0.41	1/8256 (0.0%)	0.94	38/11168 (0.3%)
1	B	0.40	0/8222	0.95	38/11122 (0.3%)
All	All	0.41	1/16478 (0.0%)	0.94	76/22290 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	ASN	CA-C	6.64	1.61	1.52

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	413	HIS	N-CA-C	8.91	123.65	112.24
1	B	893	GLY	N-CA-C	8.72	126.75	111.57
1	B	413	HIS	N-CA-C	8.18	122.70	112.24
1	A	987	ALA	N-CA-C	-8.05	103.24	113.23
1	B	81	LYS	N-CA-C	-7.95	96.72	109.76
1	A	574	GLN	N-CA-C	7.88	121.70	112.72
1	B	173	ILE	N-CA-C	7.84	120.39	108.71
1	B	51	ALA	N-CA-C	-7.80	104.37	114.04
1	B	574	GLN	N-CA-C	7.67	121.24	112.57
1	A	893	GLY	N-CA-C	7.64	131.28	113.18
1	B	817	VAL	N-CA-C	-7.53	105.87	113.47
1	B	791	THR	N-CA-C	-7.42	100.95	110.53
1	A	173	ILE	N-CA-C	7.39	120.11	108.87
1	A	791	THR	N-CA-C	-7.34	101.06	110.53
1	B	987	ALA	N-CA-C	-7.25	103.10	112.23
1	A	51	ALA	N-CA-C	-7.12	104.72	113.41
1	B	88	LYS	N-CA-C	6.81	119.28	111.11
1	B	173	ILE	O-C-N	6.70	130.04	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	582	VAL	N-CA-C	6.66	118.38	108.46
1	B	305	ARG	N-CA-C	-6.64	105.18	113.28
1	B	173	ILE	CA-C-N	6.63	134.21	121.54
1	B	173	ILE	C-N-CA	6.63	134.21	121.54
1	B	612	GLY	N-CA-C	6.53	123.03	111.73
1	B	524	MSE	N-CA-C	6.39	119.51	110.50
1	A	619	LEU	N-CA-C	-6.31	105.06	112.89
1	A	177	TYR	N-CA-C	-6.24	100.13	110.17
1	A	779	ALA	N-CA-C	-6.23	105.62	113.72
1	A	790	ALA	N-CA-C	6.07	119.16	110.24
1	B	432	ILE	N-CA-C	-5.99	98.51	107.37
1	A	524	MSE	N-CA-C	5.93	118.86	110.50
1	B	749	ARG	N-CA-C	5.88	117.11	109.64
1	A	580	ASP	N-CA-C	5.86	123.28	110.80
1	B	779	ALA	N-CA-C	-5.83	106.14	113.72
1	A	489	ILE	N-CA-C	5.82	117.25	110.62
1	A	612	GLY	N-CA-C	5.81	121.78	111.73
1	B	790	ALA	N-CA-C	5.80	118.77	110.24
1	B	565	GLU	N-CA-C	-5.80	105.09	111.82
1	A	81	LYS	N-CA-C	-5.75	99.87	109.24
1	A	467	TYR	N-CA-C	5.69	117.18	110.97
1	A	432	ILE	N-CA-C	-5.64	98.84	106.85
1	A	426	ARG	N-CA-C	5.61	117.48	111.36
1	B	618	GLY	N-CA-C	5.58	121.84	112.85
1	B	467	TYR	N-CA-C	5.55	117.02	110.97
1	A	565	GLU	N-CA-C	-5.52	105.42	111.82
1	A	378	ASN	N-CA-C	-5.47	102.43	110.52
1	A	903	GLN	N-CA-C	-5.47	105.48	111.82
1	B	619	LEU	N-CA-C	-5.44	106.14	112.89
1	A	618	GLY	N-CA-C	5.41	121.55	112.85
1	A	525	TYR	N-CA-C	5.39	119.44	112.86
1	A	191	SER	N-CA-C	5.39	119.84	113.16
1	B	82	ASN	CA-C-N	5.34	125.41	119.32
1	B	82	ASN	C-N-CA	5.34	125.41	119.32
1	B	800	GLY	N-CA-C	5.34	120.25	112.55
1	B	665	GLU	N-CA-C	-5.33	106.56	113.16
1	A	632	GLU	N-CA-C	-5.31	105.57	111.36
1	B	580	ASP	N-CA-C	5.29	122.07	110.80
1	B	539	ASP	N-CA-C	5.28	119.56	113.38
1	A	579	TRP	CA-C-N	5.26	131.58	121.54
1	A	579	TRP	C-N-CA	5.26	131.58	121.54
1	B	177	TYR	N-CA-C	-5.25	101.73	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	ALA	N-CA-C	-5.24	106.39	112.89
1	A	492	GLU	N-CA-C	-5.24	105.65	111.36
1	A	892	ARG	N-CA-C	5.20	117.85	110.10
1	B	624	ARG	N-CA-C	5.19	118.89	112.24
1	B	405	ASN	N-CA-C	5.15	118.84	112.24
1	A	82	ASN	CA-C-N	5.15	125.19	119.32
1	A	82	ASN	C-N-CA	5.15	125.19	119.32
1	A	946	VAL	N-CA-C	5.15	114.65	108.06
1	A	173	ILE	O-C-N	5.11	128.75	122.83
1	A	246	GLN	N-CA-C	-5.10	100.20	108.52
1	B	192	LYS	N-CA-C	5.10	118.82	112.59
1	A	214	VAL	N-CA-C	5.09	115.91	108.58
1	B	765	GLY	N-CA-C	-5.08	108.23	115.30
1	A	516	TYR	N-CA-C	5.07	116.81	111.28
1	B	332	TYR	N-CA-C	-5.04	103.00	110.46
1	B	625	GLU	N-CA-C	-5.01	103.45	109.72

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	8064	0	7787	162	0
1	B	8034	0	7782	152	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	563	0	0	8	0
5	B	574	0	0	14	0
All	All	17243	0	15569	314	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 10.

All (314) 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:173:ILE:HG13	1:A:174:SER:N	1.77	1.00
1:B:431:MSE:HE3	1:B:476:ILE:CG1	1.93	0.97
1:B:723:THR:HG22	1:B:725:LEU:H	1.25	0.95
1:A:714:ASN:HD21	1:A:736:GLN:HE21	1.12	0.94
1:B:431:MSE:HE3	1:B:476:ILE:HG13	1.49	0.93
1:B:1004:GLN:H	1:B:1004:GLN:NE2	1.65	0.93
1:B:1004:GLN:H	1:B:1004:GLN:HE21	0.96	0.91
1:A:1004:GLN:H	1:A:1004:GLN:HE21	1.15	0.89
1:A:723:THR:HG23	1:A:725:LEU:H	1.43	0.84
1:B:431:MSE:CE	1:B:476:ILE:HG13	2.06	0.84
1:B:356:ARG:HB2	1:B:368:ASN:HD21	1.41	0.83
1:B:1004:GLN:HE21	1:B:1004:GLN:N	1.75	0.83
1:B:836:LYS:HB2	1:B:838:GLN:HE21	1.45	0.82
1:B:431:MSE:HE2	1:B:475:ALA:HB3	1.59	0.82
1:A:1004:GLN:H	1:A:1004:GLN:NE2	1.80	0.80
1:B:60:GLY:H	1:B:422:GLN:HE22	1.29	0.80
1:B:788:ARG:HH11	1:B:989:GLN:HE21	1.30	0.80
1:B:579:TRP:HE1	1:B:617:ASN:HD22	1.30	0.79
1:B:60:GLY:H	1:B:422:GLN:NE2	1.80	0.78
1:A:723:THR:HG21	5:A:1542:HOH:O	1.82	0.78
1:B:723:THR:HG21	5:B:1545:HOH:O	1.83	0.77
1:A:356:ARG:HB2	1:A:368:ASN:HD21	1.49	0.76
1:B:431:MSE:HE3	1:B:476:ILE:HG12	1.66	0.76
1:A:579:TRP:HE1	1:A:617:ASN:HD22	1.30	0.76
1:B:964:VAL:HG23	5:B:1572:HOH:O	1.85	0.75
1:A:947:PHE:HB3	1:A:1019:TYR:HB2	1.69	0.75
1:A:379:ARG:HD2	1:A:401:MSE:HE1	1.68	0.74
1:A:834:ASN:HD21	1:A:838:GLN:HB2	1.54	0.72
1:A:640:ILE:HD12	1:A:663:LEU:HD21	1.71	0.72
1:A:483:ASN:ND2	1:A:484:GLU:HG2	2.06	0.71
1:A:788:ARG:HH11	1:A:989:GLN:HE21	1.38	0.71
1:B:296:LEU:HG	1:B:318:ILE:HD11	1.73	0.70
1:A:357:THR:H	1:A:368:ASN:ND2	1.90	0.70
1:A:118:ILE:HG12	1:A:608:ILE:HD11	1.72	0.69
1:A:173:ILE:HG13	1:A:174:SER:H	1.52	0.69
1:B:379:ARG:HD2	1:B:401:MSE:HE1	1.73	0.69
1:A:878:PHE:CE1	1:A:880:MSE:HE2	2.27	0.69
1:A:965:LEU:HD21	1:A:976:GLU:H	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:880:MSE:CE	1:B:938:LEU:HD23	2.23	0.68
1:A:528:VAL:HG13	1:A:566:VAL:HG21	1.76	0.68
1:B:357:THR:H	1:B:368:ASN:ND2	1.92	0.67
1:A:357:THR:H	1:A:368:ASN:HD22	1.42	0.67
1:A:579:TRP:CZ2	1:A:580:ASP:OD1	2.48	0.67
1:A:878:PHE:HE1	1:A:880:MSE:HE2	1.59	0.66
1:B:356:ARG:CB	1:B:368:ASN:HD21	2.07	0.65
1:A:478:ILE:HD13	1:A:506:PRO:HD2	1.77	0.65
1:A:1004:GLN:HE21	1:A:1004:GLN:N	1.93	0.65
1:A:914:VAL:HA	1:A:917:MSE:HE2	1.78	0.64
1:B:178:VAL:HG13	1:B:185:LEU:HB2	1.79	0.64
1:A:378:ASN:OD1	1:A:410:ARG:HD3	1.98	0.64
1:A:723:THR:HG22	1:A:726:VAL:H	1.63	0.64
1:B:893:GLY:HA3	1:B:910:TYR:CE2	2.33	0.64
1:B:385:LEU:HB2	5:B:1256:HOH:O	1.98	0.64
1:A:832:ILE:HG22	1:A:840:VAL:HB	1.80	0.63
1:A:527:SER:O	1:A:531:ILE:HG12	1.99	0.63
1:A:287:LEU:O	1:A:295:VAL:HG22	1.99	0.63
1:A:723:THR:CG2	1:A:726:VAL:H	2.12	0.63
1:A:684:THR:C	1:A:685:LYS:HD2	2.24	0.62
1:B:1011:LYS:HG2	5:B:1459:HOH:O	2.00	0.62
1:A:444:TYR:OH	1:A:484:GLU:HB2	2.00	0.62
1:B:828:VAL:HG13	1:B:845:PHE:HB2	1.81	0.62
1:A:623:VAL:HG23	1:A:625:GLU:HG3	1.81	0.61
1:B:71:LEU:HD11	1:B:240:LEU:HD13	1.83	0.61
1:B:357:THR:H	1:B:368:ASN:HD22	1.46	0.61
1:A:180:VAL:HG23	1:A:185:LEU:HD11	1.81	0.61
1:B:555:ASN:H	1:B:925:GLN:NE2	1.99	0.61
1:A:173:ILE:CG1	1:A:174:SER:N	2.56	0.60
1:B:59:PRO:HA	1:B:422:GLN:HE21	1.67	0.60
1:A:71:LEU:HD11	1:A:240:LEU:HD13	1.84	0.59
1:A:670:TRP:HE1	1:A:685:LYS:NZ	1.99	0.59
1:B:834:ASN:HD21	1:B:838:GLN:HB2	1.67	0.59
1:A:714:ASN:ND2	1:A:736:GLN:HE21	1.92	0.59
1:B:176:TYR:CD1	1:B:212:LEU:HD12	2.37	0.59
1:B:719:ARG:HD3	1:B:721:GLU:O	2.02	0.59
1:A:873:ARG:HD3	1:A:986:ASP:OD1	2.03	0.59
1:B:180:VAL:HG23	1:B:185:LEU:HD11	1.85	0.59
1:B:561:LYS:O	1:B:565:GLU:HG3	2.02	0.59
1:B:894:ASP:O	1:B:895:HIS:HB3	2.03	0.59
1:A:296:LEU:HG	1:A:318:ILE:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:THR:HG22	5:A:1458:HOH:O	2.03	0.59
1:B:667:ILE:HD11	1:B:720:LYS:HE3	1.83	0.58
1:B:378:ASN:OD1	1:B:410:ARG:HD3	2.03	0.58
1:A:356:ARG:CB	1:A:368:ASN:HD21	2.16	0.58
1:B:173:ILE:CG1	1:B:174:SER:N	2.67	0.58
1:B:887:VAL:HG22	1:B:938:LEU:HD13	1.86	0.58
1:A:759:VAL:HB	1:A:769:SER:HB3	1.86	0.57
1:B:580:ASP:O	1:B:618:GLY:HA2	2.03	0.57
1:B:784:LEU:H	1:B:814:GLN:NE2	2.03	0.57
1:B:880:MSE:HE3	1:B:938:LEU:HD23	1.87	0.57
1:B:118:ILE:HG12	1:B:608:ILE:HD11	1.86	0.57
1:B:364:ARG:HD3	1:B:571:PRO:O	2.04	0.57
1:B:723:THR:HG23	1:B:724:PRO:HD2	1.87	0.57
1:B:153:THR:HG23	1:B:207:GLU:HG3	1.86	0.56
1:A:784:LEU:HD23	1:A:832:ILE:HG12	1.85	0.56
1:B:173:ILE:HG13	1:B:174:SER:N	2.20	0.56
1:B:723:THR:HG22	1:B:725:LEU:N	2.08	0.56
1:B:538:LYS:HE2	5:B:1539:HOH:O	2.05	0.56
1:B:635:LYS:O	1:B:638:GLN:HG2	2.05	0.56
1:A:561:LYS:O	1:A:565:GLU:HG3	2.05	0.56
1:A:635:LYS:O	1:A:638:GLN:HG2	2.06	0.56
1:A:784:LEU:H	1:A:814:GLN:NE2	2.04	0.56
1:A:378:ASN:HB3	1:A:412:SER:OG	2.07	0.55
1:B:356:ARG:CA	1:B:368:ASN:HD21	2.20	0.55
1:B:528:VAL:HG13	1:B:566:VAL:HG21	1.88	0.55
1:B:527:SER:O	1:B:531:ILE:HG12	2.06	0.55
1:A:850:ASP:OD2	1:A:852:ASN:HB2	2.05	0.55
1:B:880:MSE:HE1	1:B:938:LEU:HD23	1.88	0.55
1:B:714:ASN:HD21	1:B:736:GLN:HE21	1.53	0.54
1:A:555:ASN:H	1:A:925:GLN:NE2	2.05	0.54
1:A:839:LYS:HD2	1:A:842:MSE:HE2	1.90	0.54
1:A:906:ARG:HD3	5:A:1566:HOH:O	2.07	0.54
1:B:1010:LYS:HB2	5:B:1114:HOH:O	2.07	0.54
1:B:173:ILE:HG13	1:B:174:SER:H	1.72	0.54
1:B:244:PRO:HG2	1:B:246:GLN:O	2.08	0.54
1:B:591:LYS:HG3	5:B:1178:HOH:O	2.08	0.54
1:A:938:LEU:HD21	1:A:981:ILE:CD1	2.38	0.53
1:A:828:VAL:CG1	1:A:845:PHE:HB2	2.39	0.53
1:A:626:PRO:HB3	1:A:630:LEU:HD23	1.90	0.53
1:A:742:ASN:O	1:A:745:THR:HG22	2.09	0.53
1:B:947:PHE:HB3	1:B:1019:TYR:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:TRP:HA	1:A:163:ARG:HD3	1.90	0.53
1:A:784:LEU:H	1:A:814:GLN:HE22	1.56	0.53
1:B:266:ILE:HD12	1:B:317:LYS:HE2	1.89	0.53
1:A:226:GLN:HG2	1:A:413:HIS:HB2	1.91	0.53
1:A:621:ASN:ND2	1:A:625:GLU:HB2	2.24	0.53
1:B:878:PHE:CE1	1:B:880:MSE:HE2	2.45	0.52
1:A:413:HIS:HA	1:A:434:GLU:OE1	2.09	0.52
1:A:795:ASN:ND2	1:A:805:ARG:HH22	2.06	0.52
1:B:894:ASP:O	1:B:894:ASP:CG	2.50	0.52
1:B:809:LEU:HA	1:B:812:LEU:HD21	1.91	0.52
1:B:226:GLN:HG2	1:B:413:HIS:HB2	1.91	0.52
1:A:762:LYS:O	1:A:816:VAL:HG21	2.09	0.52
1:B:759:VAL:HB	1:B:769:SER:HB3	1.92	0.51
1:A:706:ASN:HB2	1:A:742:ASN:HD22	1.75	0.51
1:A:887:VAL:HG21	1:A:917:MSE:CE	2.40	0.51
1:B:300:ILE:HG12	1:B:313:PHE:CE1	2.45	0.51
1:A:646:ASP:OD2	1:A:648:LYS:HG2	2.10	0.51
1:A:531:ILE:HD13	1:A:544:PHE:CE1	2.45	0.51
1:A:914:VAL:HA	1:A:917:MSE:CE	2.40	0.51
1:A:869:LYS:HA	5:A:1431:HOH:O	2.10	0.51
1:B:379:ARG:HD2	1:B:401:MSE:CE	2.41	0.51
1:A:49:PRO:HG3	1:A:242:SER:O	2.11	0.50
1:A:938:LEU:HD21	1:A:981:ILE:HD12	1.92	0.50
1:A:153:THR:OG1	1:A:207:GLU:HG3	2.11	0.50
1:B:488:GLY:O	1:B:492:GLU:HG3	2.11	0.50
1:A:632:GLU:HA	1:A:904:SER:HB3	1.92	0.50
1:B:254:SER:HB3	1:B:268:ASN:HB2	1.92	0.50
1:B:363:GLY:HA3	1:B:572:MSE:HE3	1.93	0.50
1:B:493:ARG:HG3	1:B:493:ARG:HH11	1.76	0.50
1:A:403:GLN:HG2	1:A:726:VAL:HG22	1.93	0.50
1:A:834:ASN:ND2	1:A:838:GLN:HB2	2.25	0.50
1:B:318:ILE:HD13	5:B:1574:HOH:O	2.12	0.50
1:B:655:LYS:HE2	1:B:657:TRP:CZ2	2.47	0.50
1:B:583:ASP:HB3	1:B:585:ASN:ND2	2.27	0.50
1:A:958:ILE:HG23	1:A:983:ILE:HD13	1.93	0.49
1:A:340:ASP:OD2	1:A:344:LYS:HB3	2.12	0.49
1:A:887:VAL:HG22	1:A:938:LEU:HD13	1.94	0.49
1:B:173:ILE:HG23	1:B:232:SER:HA	1.93	0.49
1:B:160:TRP:HA	1:B:163:ARG:HD3	1.95	0.49
1:A:477:VAL:HG23	1:A:478:ILE:HG12	1.94	0.49
1:A:727:ASP:HB2	5:A:1362:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:ARG:HB2	1:B:368:ASN:ND2	2.19	0.49
1:B:398:ILE:HD13	1:B:398:ILE:O	2.12	0.49
1:A:356:ARG:CA	1:A:368:ASN:HD21	2.25	0.49
1:A:817:VAL:HG12	1:A:829:ARG:O	2.13	0.49
1:A:639:ASN:O	1:A:640:ILE:HD13	2.13	0.49
1:A:69:MSE:HE2	1:A:240:LEU:HD22	1.95	0.48
1:A:82:ASN:C	1:A:82:ASN:OD1	2.55	0.48
1:B:23:LEU:HD13	1:B:27:LEU:HD13	1.94	0.48
1:B:431:MSE:HE2	1:B:475:ALA:CB	2.36	0.48
1:B:408:MSE:SE	1:B:432:ILE:HG13	2.63	0.48
1:A:282:SER:HB3	1:A:301:ASN:HD22	1.78	0.48
1:A:871:MSE:HG3	1:A:1009:VAL:HG22	1.95	0.48
1:B:795:ASN:ND2	1:B:805:ARG:HH22	2.11	0.48
1:B:893:GLY:HA3	1:B:910:TYR:CD2	2.48	0.48
1:B:110:GLU:HA	1:B:114:TYR:O	2.14	0.48
1:B:958:ILE:HG23	1:B:983:ILE:HD13	1.96	0.48
1:B:628:PRO:HD3	1:B:919:HIS:CE1	2.49	0.48
1:B:668:LEU:HD11	1:B:715:LEU:HD22	1.96	0.48
1:A:40:LYS:HG2	1:A:197:TRP:CE2	2.49	0.47
1:A:933:VAL:HG21	1:A:956:PHE:HD2	1.79	0.47
1:B:646:ASP:HB3	1:B:651:LYS:HB3	1.94	0.47
1:A:133:PHE:CG	1:A:141:PRO:HG3	2.48	0.47
1:A:579:TRP:CE2	1:A:580:ASP:OD1	2.68	0.47
1:B:43:PRO:HB2	1:B:468:GLU:HG3	1.96	0.47
1:B:49:PRO:HG3	1:B:242:SER:O	2.13	0.47
1:A:509:TYR:CZ	1:A:511:ARG:HB2	2.50	0.47
1:B:71:LEU:CD1	1:B:240:LEU:HD13	2.44	0.47
1:A:818:SER:HB3	1:A:829:ARG:HB3	1.95	0.47
1:A:828:VAL:HG13	1:A:845:PHE:HB2	1.96	0.47
1:A:977:ARG:HG3	1:A:977:ARG:HH11	1.80	0.47
1:B:74:LYS:NZ	1:B:104:ASN:HD21	2.11	0.47
1:B:667:ILE:HD11	1:B:720:LYS:HG2	1.96	0.47
1:B:788:ARG:NH1	1:B:989:GLN:HE21	2.06	0.47
1:B:833:LEU:HD22	1:B:833:LEU:N	2.29	0.47
1:B:671:ASN:OD1	1:B:673:LYS:HG3	2.15	0.47
1:A:948:MSE:HG2	1:A:1018:LEU:HD22	1.96	0.47
1:B:746:THR:HB	1:B:749:ARG:HD2	1.96	0.47
1:A:887:VAL:HG21	1:A:917:MSE:HE1	1.97	0.47
1:B:882:ASP:OD2	1:B:979:GLY:HA2	2.15	0.47
1:A:180:VAL:CG2	1:A:185:LEU:HD11	2.46	0.46
1:A:244:PRO:HG2	1:A:246:GLN:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:619:LEU:HB3	1:A:630:LEU:HD13	1.96	0.46
1:B:620:VAL:HG12	1:B:626:PRO:HA	1.98	0.46
1:A:880:MSE:HE3	1:A:983:ILE:HG13	1.96	0.46
1:B:965:LEU:HD12	5:B:1135:HOH:O	2.16	0.46
1:A:257:LEU:HA	1:A:264:GLU:O	2.16	0.46
1:A:285:TYR:CD1	1:A:285:TYR:C	2.94	0.46
1:B:385:LEU:HD12	5:B:1256:HOH:O	2.14	0.46
1:B:834:ASN:ND2	1:B:838:GLN:HB2	2.28	0.46
1:A:820:LYS:NZ	1:A:820:LYS:HB3	2.31	0.46
1:A:655:LYS:HE2	1:A:657:TRP:CZ2	2.51	0.45
1:B:795:ASN:HD21	1:B:805:ARG:HH12	1.64	0.45
1:B:938:LEU:HD21	1:B:981:ILE:CD1	2.46	0.45
1:B:892:ARG:HD2	1:B:902:ASN:HB2	1.97	0.45
1:B:311:ILE:N	1:B:311:ILE:HD12	2.31	0.45
1:A:511:ARG:NE	1:A:511:ARG:HA	2.31	0.45
1:A:670:TRP:HE1	1:A:685:LYS:HZ2	1.63	0.45
1:A:766:ALA:HB1	1:A:782:ILE:O	2.17	0.45
1:A:109:TRP:CE2	1:A:232:SER:HB2	2.52	0.45
1:B:40:LYS:HG2	1:B:197:TRP:CE2	2.52	0.45
1:B:385:LEU:HD22	5:B:1275:HOH:O	2.17	0.45
1:B:742:ASN:O	1:B:745:THR:HG22	2.17	0.44
1:B:944:GLU:HG2	1:B:1022:LYS:HG3	1.99	0.44
1:A:124:TYR:CE2	1:A:222:TYR:HA	2.53	0.44
1:A:483:ASN:O	1:A:484:GLU:C	2.60	0.44
1:A:921:TYR:O	1:A:972:ILE:HD11	2.17	0.44
1:B:211:ALA:C	1:B:212:LEU:HD22	2.42	0.44
1:A:456:LEU:C	1:A:456:LEU:HD13	2.43	0.44
1:A:882:ASP:OD2	1:A:979:GLY:HA2	2.17	0.44
1:B:858:ARG:HG2	1:B:858:ARG:HH11	1.81	0.44
1:B:116:THR:HG21	1:B:608:ILE:HD12	2.00	0.44
1:A:705:PRO:HG2	1:A:708:VAL:HG22	1.99	0.44
1:A:261:LYS:O	1:A:263:LYS:HG2	2.16	0.44
1:B:388:THR:HB	5:B:1256:HOH:O	2.17	0.44
1:A:933:VAL:HG21	1:A:956:PHE:CD2	2.52	0.43
1:B:493:ARG:HG3	1:B:493:ARG:NH1	2.33	0.43
1:B:791:THR:HA	1:B:925:GLN:HB2	2.00	0.43
1:B:977:ARG:HG3	1:B:977:ARG:HH11	1.82	0.43
1:A:300:ILE:HG12	1:A:313:PHE:CE1	2.53	0.43
1:B:285:TYR:CD1	1:B:285:TYR:C	2.96	0.43
1:B:788:ARG:O	1:B:789:PRO:C	2.62	0.43
1:A:273:VAL:O	1:A:308:SER:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:TYR:CE2	1:A:511:ARG:HB2	2.54	0.43
1:A:71:LEU:CD1	1:A:240:LEU:HD13	2.49	0.43
1:A:477:VAL:O	1:A:478:ILE:HD13	2.19	0.43
1:A:178:VAL:HG23	1:A:212:LEU:CD2	2.49	0.43
1:B:137:PRO:HG3	1:B:222:TYR:CE2	2.54	0.43
1:B:413:HIS:ND1	1:B:413:HIS:N	2.66	0.43
1:B:839:LYS:O	1:B:867:ILE:HD12	2.19	0.43
1:A:254:SER:HB3	1:A:268:ASN:HB2	2.01	0.42
1:A:551:HIS:CG	1:A:997:CYS:HB3	2.55	0.42
1:A:880:MSE:CE	1:A:983:ILE:HG13	2.49	0.42
1:B:642:ALA:HA	1:B:653:CYS:O	2.19	0.42
1:A:399:ARG:O	1:A:403:GLN:HG3	2.19	0.42
1:B:90:PHE:HA	1:B:95:TYR:CG	2.54	0.42
1:B:356:ARG:HA	1:B:368:ASN:HD21	1.84	0.42
1:B:984:HIS:HD2	5:B:1071:HOH:O	2.02	0.42
1:A:432:ILE:HG12	1:A:478:ILE:HB	2.01	0.42
1:A:719:ARG:HG2	5:A:1494:HOH:O	2.18	0.42
1:A:668:LEU:HB2	1:A:717:TRP:CZ3	2.54	0.42
1:B:772:LEU:HD13	1:B:1020:PRO:HB2	2.00	0.42
1:B:788:ARG:HA	1:B:873:ARG:HH21	1.85	0.42
1:A:110:GLU:HA	1:A:114:TYR:O	2.20	0.42
1:A:178:VAL:HG13	1:A:185:LEU:HB2	2.01	0.42
1:A:890:LEU:HD22	5:A:1374:HOH:O	2.19	0.42
1:B:587:ARG:HB2	1:B:597:TRP:CZ3	2.55	0.42
1:A:151:ARG:HG3	1:A:211:ALA:HB2	2.02	0.42
1:A:513:GLU:HA	5:A:1057:HOH:O	2.18	0.42
1:A:640:ILE:HD12	1:A:663:LEU:CD2	2.44	0.42
1:B:404:HIS:CD2	1:B:630:LEU:HG	2.55	0.42
1:B:685:LYS:HB2	1:B:685:LYS:NZ	2.35	0.42
1:B:723:THR:HG23	1:B:724:PRO:CD	2.48	0.42
1:A:141:PRO:O	1:A:145:ASN:HB2	2.19	0.42
1:A:768:SER:HA	1:A:781:PRO:HB3	2.02	0.42
1:A:823:LYS:HD3	1:A:823:LYS:O	2.20	0.42
1:A:484:GLU:HA	1:A:511:ARG:CG	2.50	0.42
1:A:893:GLY:N	1:A:906:ARG:O	2.51	0.42
1:B:450:ALA:HB2	1:B:485:ALA:O	2.20	0.42
1:A:255:ALA:HB1	1:A:355:PHE:CD1	2.55	0.41
1:B:938:LEU:O	1:B:945:GLY:HA3	2.20	0.41
1:A:211:ALA:C	1:A:212:LEU:HD23	2.44	0.41
1:B:632:GLU:HA	1:B:904:SER:HB3	2.02	0.41
1:B:880:MSE:CE	1:B:983:ILE:HG13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:ILE:CD1	1:A:506:PRO:HB3	2.51	0.41
1:A:431:MSE:HB2	1:A:476:ILE:HA	2.03	0.41
1:A:791:THR:HA	1:A:925:GLN:HB2	2.01	0.41
1:A:831:GLU:HG2	1:A:842:MSE:SE	2.71	0.41
1:A:839:LYS:HD2	1:A:842:MSE:CE	2.50	0.41
1:B:304:SER:HB2	5:B:1312:HOH:O	2.19	0.41
1:A:408:MSE:SE	1:A:432:ILE:HG13	2.70	0.41
1:B:784:LEU:H	1:B:814:GLN:HE22	1.65	0.41
1:A:782:ILE:HA	1:A:878:PHE:HB3	2.02	0.41
1:B:628:PRO:HB3	1:B:896:GLU:HB3	2.03	0.41
1:B:762:LYS:O	1:B:816:VAL:HG21	2.21	0.41
1:A:620:VAL:HG12	1:A:626:PRO:HA	2.02	0.41
1:B:403:GLN:HB3	1:B:730:TRP:CZ2	2.56	0.41
1:B:878:PHE:HE1	1:B:880:MSE:HE2	1.86	0.41
1:A:74:LYS:NZ	1:A:104:ASN:HD21	2.19	0.41
1:A:965:LEU:HD12	1:A:965:LEU:O	2.21	0.41
1:B:758:PHE:HA	1:B:769:SER:O	2.21	0.41
1:A:807:ALA:HB3	1:A:809:LEU:HG	2.03	0.40
1:A:884:TYR:HB3	1:A:938:LEU:HG	2.03	0.40
1:B:392:GLU:CD	1:B:392:GLU:H	2.29	0.40
1:B:413:HIS:HA	1:B:434:GLU:OE1	2.20	0.40
1:A:691:PRO:O	1:A:692:HIS:HB2	2.21	0.40
1:A:880:MSE:CE	1:A:938:LEU:HD23	2.52	0.40
1:B:483:ASN:O	1:B:484:GLU:C	2.64	0.40
1:A:178:VAL:HG23	1:A:212:LEU:HD22	2.02	0.40
1:A:977:ARG:HG3	1:A:977:ARG:NH1	2.36	0.40
1:B:913:THR:O	1:B:917:MSE:HG3	2.21	0.40
1:A:580:ASP:O	1:A:618:GLY:HA2	2.20	0.40
1:B:635:LYS:HE3	1:B:734:TYR:O	2.22	0.40
1:B:963:ASP:OD2	1:B:984:HIS:HE1	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1001/1010 (99%)	954 (95%)	41 (4%)	6 (1%)	21	18
1	B	998/1010 (99%)	948 (95%)	43 (4%)	7 (1%)	18	15
All	All	1999/2020 (99%)	1902 (95%)	84 (4%)	13 (1%)	18	15

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	412	SER
1	B	412	SER
1	A	893	GLY
1	B	513	GLU
1	B	895	HIS
1	B	174	SER
1	A	82	ASN
1	A	174	SER
1	A	484	GLU
1	A	580	ASP
1	B	82	ASN
1	B	865	THR
1	B	518	THR

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	854/840 (102%)	839 (98%)	15 (2%)	51	60
1	B	852/840 (101%)	832 (98%)	20 (2%)	44	51
All	All	1706/1680 (102%)	1671 (98%)	35 (2%)	47	54

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	ILE
1	A	174	SER
1	A	212	LEU
1	A	240	LEU
1	A	256	SER
1	A	380	HIS
1	A	413	HIS
1	A	471	LYS
1	A	546	LEU
1	A	580	ASP
1	A	755	GLU
1	A	820	LYS
1	A	821	GLU
1	A	976	GLU
1	A	1004	GLN
1	B	27	LEU
1	B	153	THR
1	B	174	SER
1	B	232	SER
1	B	380	HIS
1	B	398	ILE
1	B	413	HIS
1	B	499	LYS
1	B	546	LEU
1	B	580	ASP
1	B	685	LYS
1	B	723	THR
1	B	767	LEU
1	B	770	LEU
1	B	828	VAL
1	B	833	LEU
1	B	850	ASP
1	B	906	ARG
1	B	941	GLN
1	B	1004	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	85	ASN
1	A	104	ASN
1	A	297	GLN

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Mol	Chain	Res	Type
1	A	301	ASN
1	A	309	ASN
1	A	368	ASN
1	A	380	HIS
1	A	403	GLN
1	A	481	GLN
1	A	490	ASN
1	A	585	ASN
1	A	639	ASN
1	A	714	ASN
1	A	744	ASN
1	A	795	ASN
1	A	811	ASN
1	A	814	GLN
1	A	838	GLN
1	A	862	GLN
1	A	925	GLN
1	A	941	GLN
1	A	955	GLN
1	A	989	GLN
1	A	1004	GLN
1	B	25	GLN
1	B	85	ASN
1	B	104	ASN
1	B	246	GLN
1	B	297	GLN
1	B	301	ASN
1	B	368	ASN
1	B	380	HIS
1	B	396	GLN
1	B	403	GLN
1	B	411	ASN
1	B	422	GLN
1	B	481	GLN
1	B	490	ASN
1	B	508	GLN
1	B	515	ASN
1	B	585	ASN
1	B	639	ASN
1	B	649	ASN
1	B	714	ASN
1	B	795	ASN

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Mol	Chain	Res	Type
1	B	811	ASN
1	B	814	GLN
1	B	838	GLN
1	B	925	GLN
1	B	929	ASN
1	B	984	HIS
1	B	989	GLN
1	B	1004	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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 ⓘ

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	983/1010 (97%)	0.12	23 (2%) 61 64	10, 24, 43, 55	0
1	B	980/1010 (97%)	0.02	23 (2%) 61 64	11, 23, 39, 58	0
All	All	1963/2020 (97%)	0.07	46 (2%) 61 64	10, 23, 41, 58	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	893	GLY	6.1
1	B	174	SER	4.6
1	B	894	ASP	4.5
1	A	174	SER	4.1
1	A	580	ASP	4.0
1	B	893	GLY	4.0
1	B	580	ASP	3.8
1	B	302	ILE	3.6
1	A	894	ASP	3.4
1	B	305	ARG	3.3
1	B	837	GLY	3.1
1	B	522	CYS	3.0
1	B	850	ASP	3.0
1	B	306	GLY	2.9
1	A	850	ASP	2.8
1	A	522	CYS	2.8
1	B	849	LEU	2.7
1	A	701	ALA	2.7
1	B	303	LYS	2.6
1	B	817	VAL	2.6
1	B	304	SER	2.6
1	A	340	ASP	2.5
1	A	828	VAL	2.5
1	A	832	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	547	CYS	2.5
1	A	697	VAL	2.4
1	B	320	GLU	2.4
1	A	305	ARG	2.3
1	A	205	GLU	2.3
1	B	647	ARG	2.3
1	A	645	SER	2.2
1	A	547	CYS	2.2
1	A	837	GLY	2.2
1	B	941	GLN	2.1
1	B	340	ASP	2.1
1	A	849	LEU	2.1
1	B	57	GLY	2.1
1	B	173	ILE	2.1
1	B	852	ASN	2.1
1	A	153	THR	2.1
1	A	702	VAL	2.1
1	A	816	VAL	2.1
1	A	681	ALA	2.1
1	A	318	ILE	2.0
1	B	811	ASN	2.0
1	A	819	LEU	2.0

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 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(Å ²)	Q<0.9
3	NA	B	3	1/1	0.92	0.08	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	1	1/1	0.95	0.03	10,10,10,10	0
2	MG	B	2	1/1	0.96	0.03	20,20,20,20	0
3	NA	A	6	1/1	0.97	0.03	21,21,21,21	0
3	NA	A	4	1/1	0.98	0.10	15,15,15,15	0
3	NA	B	5	1/1	0.98	0.03	18,18,18,18	0
4	CL	A	7	1/1	0.99	0.06	12,12,12,12	0
4	CL	B	8	1/1	0.99	0.13	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.