



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:29 am GMT

PDB ID : 1UWI
Title : CRYSTAL STRUCTURE OF MUTATED BETA-GLYCOSIDASE FROM
SULFOLOBUS SOLFATARICUS, WORKING AT MODERATE TEMPER-
ATURE
Authors : Isorna, P.; Polaina, J.; Sanz-Aparicio, J.
Deposited on : 2004-02-05
Resolution : 2.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

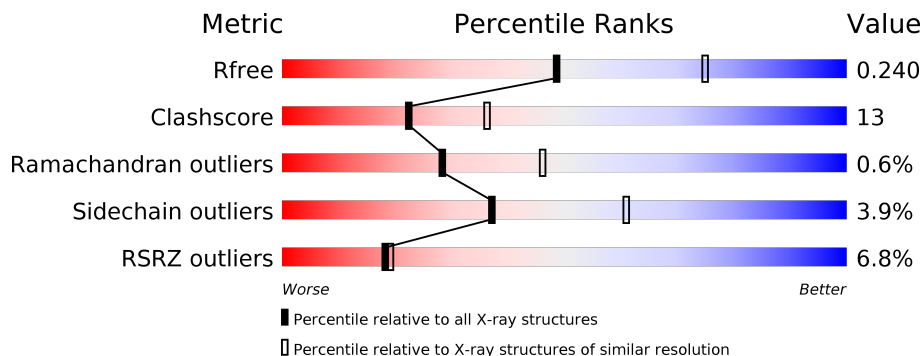
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4993 (2.58-2.50)
Clashscore	112137	5755 (2.58-2.50)
Ramachandran outliers	110173	5652 (2.58-2.50)
Sidechain outliers	110143	5654 (2.58-2.50)
RSRZ outliers	101464	5026 (2.58-2.50)

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	489	<div> <div>7%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div>.</div> </div> </div>
1	B	489	<div> <div>8%</div> <div> <div></div> <div>76%</div> <div>21%</div> <div>.</div> </div> </div>
1	C	489	<div> <div>8%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>.</div> </div> </div>
1	D	489	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>19%</div> <div>.</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16494 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	489	Total	C	N	O	S	0	0	0
			4017	2573	693	739	12			
1	B	489	Total	C	N	O	S	0	0	0
			4017	2573	693	739	12			
1	C	489	Total	C	N	O	S	0	0	0
			4017	2573	693	739	12			
1	D	489	Total	C	N	O	S	0	0	0
			4017	2573	693	739	12			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	LEU	PRO	ENGINEERED MUTATION	UNP P22498
A	68	ASN	ASP	ENGINEERED MUTATION	UNP P22498
A	331	GLY	GLU	ENGINEERED MUTATION	UNP P22498
A	459	SER	ALA	ENGINEERED MUTATION	UNP P22498
B	29	LEU	PRO	ENGINEERED MUTATION	UNP P22498
B	68	ASN	ASP	ENGINEERED MUTATION	UNP P22498
B	331	GLY	GLU	ENGINEERED MUTATION	UNP P22498
B	459	SER	ALA	ENGINEERED MUTATION	UNP P22498
C	29	LEU	PRO	ENGINEERED MUTATION	UNP P22498
C	68	ASN	ASP	ENGINEERED MUTATION	UNP P22498
C	331	GLY	GLU	ENGINEERED MUTATION	UNP P22498
C	459	SER	ALA	ENGINEERED MUTATION	UNP P22498
D	29	LEU	PRO	ENGINEERED MUTATION	UNP P22498
D	68	ASN	ASP	ENGINEERED MUTATION	UNP P22498
D	331	GLY	GLU	ENGINEERED MUTATION	UNP P22498
D	459	SER	ALA	ENGINEERED MUTATION	UNP P22498

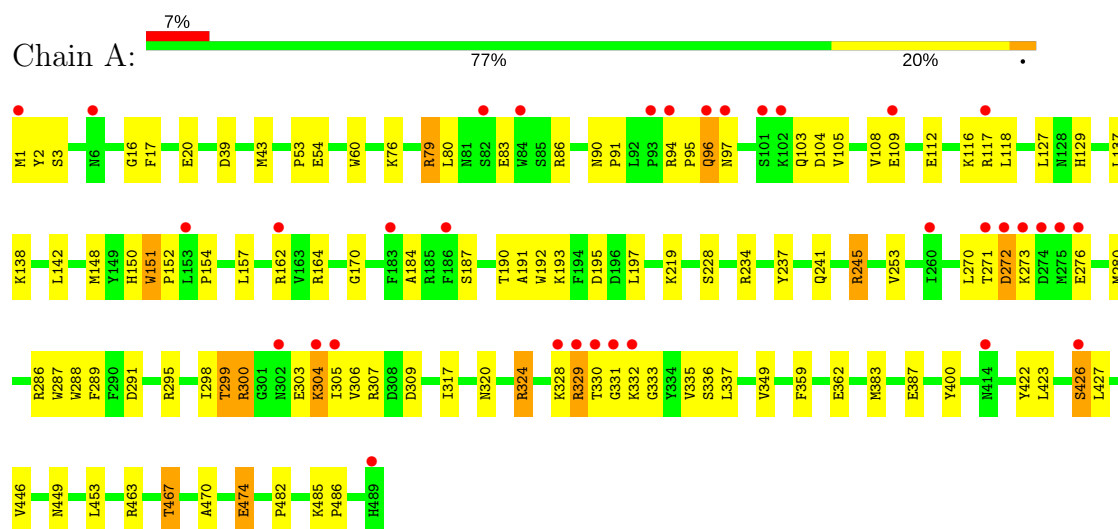
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	128	Total 128	O 128	0	0
2	B	102	Total 102	O 102	0	0
2	C	81	Total 81	O 81	0	0
2	D	115	Total 115	O 115	0	0

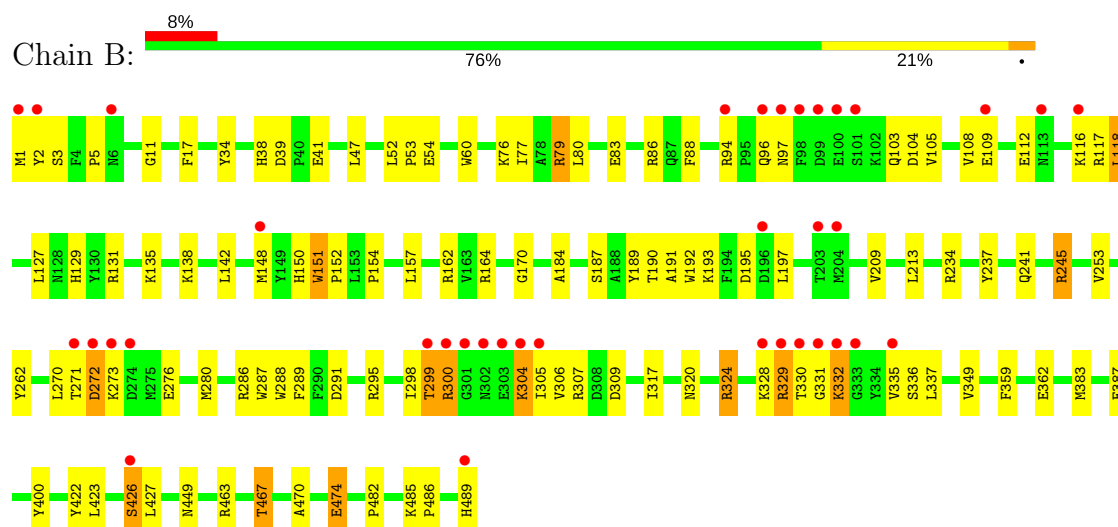
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

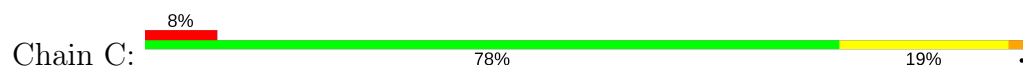
• Molecule 1: BETA-GALACTOSIDASE

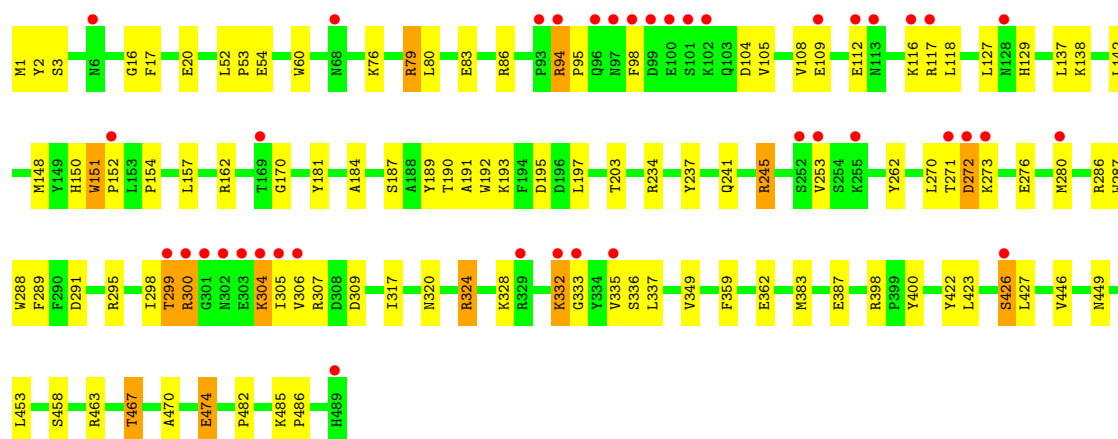


• Molecule 1: BETA-GALACTOSIDASE

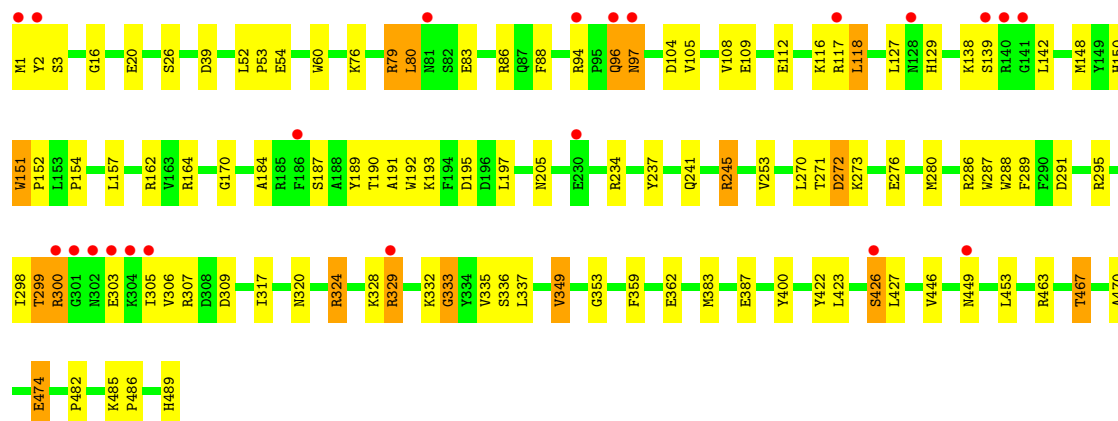
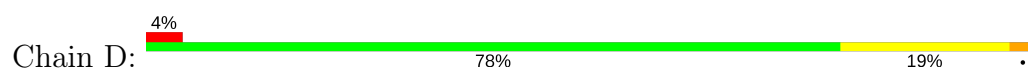


• Molecule 1: BETA-GALACTOSIDASE





• Molecule 1: BETA-GALACTOSIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.08Å 132.43Å 219.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.44 – 2.55 28.44 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.2 (28.44-2.55) 99.2 (28.44-2.50)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.51Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.209 , 0.241 0.209 , 0.240	Depositor DCC
R_{free} test set	5325 reflections (7.09%)	DCC
Wilson B-factor (Å ²)	32.0	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 52.7	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	16494	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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

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	0.36	0/4145	0.60	1/5629 (0.0%)
1	B	0.36	0/4145	0.60	1/5629 (0.0%)
1	C	0.36	0/4145	0.60	1/5629 (0.0%)
1	D	0.36	0/4145	0.60	1/5629 (0.0%)
All	All	0.36	0/16580	0.60	4/22516 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	426	SER	N-CA-C	5.39	125.56	111.00
1	A	426	SER	N-CA-C	5.32	125.36	111.00
1	B	426	SER	N-CA-C	5.26	125.21	111.00
1	D	426	SER	N-CA-C	5.22	125.10	111.00

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	4017	0	3802	111	0
1	B	4017	0	3802	102	0
1	C	4017	0	3802	97	0
1	D	4017	0	3802	102	0
2	A	128	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	102	0	0	5	0
2	C	81	0	0	2	0
2	D	115	0	0	4	0
All	All	16494	0	15208	410	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 (410) 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:B:305:ILE:HG22	1:B:306:VAL:H	1.43	0.83
1:A:305:ILE:HG22	1:A:306:VAL:H	1.40	0.83
1:C:305:ILE:HG22	1:C:306:VAL:H	1.44	0.83
1:A:192:TRP:HA	1:A:253:VAL:HG11	1.62	0.82
1:D:305:ILE:HG22	1:D:306:VAL:H	1.43	0.82
1:C:192:TRP:HA	1:C:253:VAL:HG11	1.62	0.81
1:D:192:TRP:HA	1:D:253:VAL:HG11	1.61	0.81
1:C:104:ASP:HA	1:C:241:GLN:HE22	1.44	0.81
1:B:192:TRP:HA	1:B:253:VAL:HG11	1.64	0.79
1:B:104:ASP:HA	1:B:241:GLN:HE22	1.46	0.78
1:D:148:MET:HE1	1:D:190:THR:HB	1.64	0.78
1:A:104:ASP:HA	1:A:241:GLN:HE22	1.47	0.78
1:D:104:ASP:HA	1:D:241:GLN:HE22	1.47	0.78
1:B:329:ARG:HD3	1:B:330:THR:N	1.99	0.78
1:C:463:ARG:HD2	2:C:2073:HOH:O	1.85	0.76
1:B:148:MET:HE1	1:B:190:THR:HB	1.67	0.75
1:D:127:LEU:HD21	1:D:193:LYS:HD3	1.69	0.75
1:A:127:LEU:HD21	1:A:193:LYS:HD3	1.68	0.74
1:B:485:LYS:HG2	2:B:2099:HOH:O	1.88	0.74
1:C:148:MET:HE1	1:C:190:THR:HB	1.69	0.73
1:B:127:LEU:HD21	1:B:193:LYS:HD3	1.69	0.73
1:A:332:LYS:HG3	1:A:333:GLY:H	1.53	0.73
1:B:241:GLN:HE21	1:B:307:ARG:HH22	1.37	0.72
1:D:241:GLN:HE21	1:D:307:ARG:HH22	1.34	0.72
1:B:76:LYS:HA	1:B:142:LEU:HD23	1.72	0.72
1:A:241:GLN:HE21	1:A:307:ARG:HH22	1.38	0.71
1:C:127:LEU:HD21	1:C:193:LYS:HD3	1.69	0.71
1:C:485:LYS:HG2	2:C:2077:HOH:O	1.90	0.71
1:B:305:ILE:HG22	1:B:306:VAL:N	2.06	0.70
1:C:76:LYS:HA	1:C:142:LEU:HD23	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:ARG:O	1:A:467:THR:HB	1.92	0.70
1:A:305:ILE:HG22	1:A:306:VAL:N	2.05	0.70
1:A:94:ARG:HB3	1:A:94:ARG:NH1	2.07	0.70
1:D:305:ILE:HG22	1:D:306:VAL:N	2.07	0.70
1:A:148:MET:HE1	1:A:190:THR:HB	1.72	0.69
1:A:299:THR:HB	1:A:304:LYS:HE3	1.74	0.69
1:A:76:LYS:HA	1:A:142:LEU:HD23	1.74	0.69
1:C:305:ILE:HG22	1:C:306:VAL:N	2.08	0.68
1:C:463:ARG:O	1:C:467:THR:HB	1.94	0.68
1:D:76:LYS:HA	1:D:142:LEU:HD23	1.75	0.68
1:D:329:ARG:HG3	1:D:329:ARG:HH11	1.57	0.68
1:B:463:ARG:O	1:B:467:THR:HB	1.94	0.67
1:C:241:GLN:HE21	1:C:307:ARG:HH22	1.40	0.67
1:A:328:LYS:HD2	1:A:337:LEU:HD21	1.77	0.67
1:B:96:GLN:HG3	1:B:97:ASN:H	1.60	0.67
1:D:463:ARG:O	1:D:467:THR:HB	1.95	0.67
1:B:328:LYS:HD2	1:B:337:LEU:HD21	1.76	0.66
1:B:105:VAL:H	1:B:241:GLN:NE2	1.95	0.64
1:A:324:ARG:HD3	1:A:362:GLU:OE1	1.97	0.64
1:B:148:MET:CE	1:B:187:SER:HA	2.27	0.64
1:C:105:VAL:H	1:C:241:GLN:NE2	1.96	0.64
1:D:324:ARG:HD3	1:D:362:GLU:OE1	1.97	0.64
1:A:105:VAL:H	1:A:241:GLN:NE2	1.95	0.64
1:D:241:GLN:NE2	1:D:307:ARG:HH12	1.95	0.63
1:C:148:MET:CE	1:C:187:SER:HA	2.28	0.63
1:D:192:TRP:CA	1:D:253:VAL:HG11	2.29	0.63
1:B:271:THR:HG22	1:B:272:ASP:N	2.14	0.63
1:A:271:THR:HG22	1:A:272:ASP:N	2.14	0.63
1:A:148:MET:CE	1:A:187:SER:HA	2.28	0.63
1:D:328:LYS:HD2	1:D:337:LEU:HD21	1.80	0.62
1:B:324:ARG:HD3	1:B:362:GLU:OE1	1.99	0.62
1:C:271:THR:HG22	1:C:272:ASP:N	2.13	0.62
1:C:328:LYS:HD2	1:C:337:LEU:HD21	1.79	0.62
1:D:96:GLN:O	1:D:97:ASN:OD1	2.17	0.62
1:B:286:ARG:NH1	2:B:2057:HOH:O	2.32	0.62
1:D:105:VAL:H	1:D:241:GLN:NE2	1.97	0.62
1:C:324:ARG:HD3	1:C:362:GLU:OE1	1.99	0.62
1:B:96:GLN:CG	1:B:97:ASN:H	2.13	0.62
1:D:148:MET:CE	1:D:187:SER:HA	2.29	0.62
1:A:241:GLN:NE2	1:A:307:ARG:HH12	1.96	0.61
1:B:241:GLN:NE2	1:B:307:ARG:HH12	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:TRP:HB2	1:C:152:PRO:HD3	1.83	0.61
1:A:109:GLU:HG3	1:A:109:GLU:O	2.00	0.60
1:D:271:THR:HG22	1:D:272:ASP:N	2.15	0.60
1:A:241:GLN:HE21	1:A:307:ARG:HH12	1.49	0.60
1:D:109:GLU:O	1:D:109:GLU:HG3	2.01	0.60
1:B:94:ARG:NH1	1:B:94:ARG:HB3	2.17	0.60
1:C:241:GLN:NE2	1:C:307:ARG:HH12	1.99	0.60
1:B:109:GLU:O	1:B:109:GLU:HG3	2.01	0.59
1:C:109:GLU:O	1:C:109:GLU:HG3	2.02	0.59
1:A:151:TRP:HB2	1:A:152:PRO:HD3	1.84	0.59
1:A:286:ARG:HD2	1:A:287:TRP:CZ3	2.37	0.59
1:B:192:TRP:CA	1:B:253:VAL:HG11	2.31	0.59
1:C:192:TRP:CA	1:C:253:VAL:HG11	2.30	0.59
1:B:241:GLN:HE21	1:B:307:ARG:HH12	1.51	0.59
1:B:286:ARG:HD2	1:B:287:TRP:CZ3	2.38	0.58
1:C:271:THR:HG21	1:C:273:LYS:NZ	2.19	0.58
1:A:148:MET:HE1	1:A:187:SER:HA	1.84	0.58
1:C:286:ARG:HD2	1:C:287:TRP:CZ3	2.38	0.58
1:D:329:ARG:HD3	1:D:333:GLY:O	2.04	0.58
1:D:117:ARG:NH1	1:D:117:ARG:HB2	2.19	0.58
1:B:271:THR:HG21	1:B:273:LYS:NZ	2.19	0.58
1:A:117:ARG:HB2	1:A:117:ARG:NH1	2.19	0.58
1:C:3:SER:HA	1:C:470:ALA:HB2	1.87	0.57
1:D:241:GLN:HE21	1:D:307:ARG:NH2	2.01	0.57
1:A:237:TYR:CE1	1:A:300:ARG:HB3	2.38	0.57
1:A:192:TRP:CA	1:A:253:VAL:HG11	2.30	0.57
1:D:151:TRP:HB2	1:D:152:PRO:HD3	1.85	0.57
1:D:241:GLN:HE21	1:D:307:ARG:HH12	1.51	0.57
1:A:3:SER:HA	1:A:470:ALA:HB2	1.86	0.57
1:A:271:THR:HG21	1:A:273:LYS:NZ	2.20	0.57
1:C:117:ARG:NH1	1:C:117:ARG:HB2	2.20	0.57
1:A:79:ARG:C	1:A:80:LEU:HD12	2.25	0.57
1:C:241:GLN:HE21	1:C:307:ARG:HH12	1.51	0.57
1:C:485:LYS:HB2	1:C:486:PRO:HD3	1.86	0.57
1:C:94:ARG:NH1	1:C:94:ARG:HB3	2.19	0.57
1:D:3:SER:HA	1:D:470:ALA:HB2	1.85	0.57
1:B:151:TRP:HB2	1:B:152:PRO:HD3	1.85	0.57
1:B:241:GLN:HE21	1:B:307:ARG:NH2	2.03	0.57
1:A:485:LYS:HB2	1:A:486:PRO:HD3	1.87	0.56
1:B:3:SER:HA	1:B:470:ALA:HB2	1.87	0.56
1:B:485:LYS:HB2	1:B:486:PRO:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:271:THR:HG21	1:D:273:LYS:NZ	2.20	0.56
1:D:286:ARG:HD2	1:D:287:TRP:CZ3	2.41	0.56
1:B:270:LEU:HD22	1:B:337:LEU:HD11	1.86	0.56
1:C:280:MET:HE1	1:C:332:LYS:O	2.06	0.55
1:D:150:HIS:O	1:D:151:TRP:HB2	2.05	0.55
1:C:79:ARG:C	1:C:80:LEU:HD12	2.27	0.55
1:A:303:GLU:HB3	1:A:305:ILE:HD11	1.87	0.55
1:B:79:ARG:C	1:B:80:LEU:HD12	2.27	0.55
1:D:286:ARG:HG3	1:D:286:ARG:HH11	1.71	0.55
1:B:117:ARG:HB2	1:B:117:ARG:NH1	2.21	0.55
1:A:330:THR:O	1:A:332:LYS:N	2.40	0.54
1:D:270:LEU:HD22	1:D:337:LEU:CD1	2.37	0.54
1:B:270:LEU:HD22	1:B:337:LEU:CD1	2.37	0.54
1:B:148:MET:HE1	1:B:187:SER:HA	1.89	0.54
1:D:79:ARG:C	1:D:80:LEU:HD12	2.28	0.54
1:B:286:ARG:HH11	1:B:286:ARG:HG3	1.73	0.54
1:A:270:LEU:HD22	1:A:337:LEU:CD1	2.38	0.54
1:B:329:ARG:HD3	1:B:330:THR:H	1.73	0.54
1:A:103:GLN:OE1	1:A:300:ARG:HD3	2.08	0.54
1:A:150:HIS:O	1:A:151:TRP:HB2	2.08	0.54
1:A:270:LEU:HD22	1:A:337:LEU:HD11	1.89	0.54
1:C:241:GLN:HE21	1:C:307:ARG:NH2	2.06	0.54
1:C:270:LEU:HD22	1:C:337:LEU:HD11	1.89	0.53
1:D:485:LYS:HB2	1:D:486:PRO:HD3	1.89	0.53
1:C:270:LEU:HD22	1:C:337:LEU:CD1	2.38	0.53
1:D:270:LEU:HD22	1:D:337:LEU:HD11	1.88	0.53
1:D:305:ILE:CG2	1:D:306:VAL:H	2.20	0.53
1:B:237:TYR:CE1	1:B:300:ARG:HB3	2.44	0.52
1:C:271:THR:HG21	1:C:273:LYS:HZ3	1.74	0.52
1:A:329:ARG:HH11	1:A:329:ARG:HG3	1.73	0.52
1:B:489:HIS:HB3	2:B:2101:HOH:O	2.08	0.52
1:A:300:ARG:HD2	1:A:300:ARG:O	2.09	0.52
1:B:148:MET:HE2	1:B:187:SER:HA	1.91	0.52
1:C:148:MET:HE2	1:C:187:SER:HA	1.91	0.52
1:A:286:ARG:HH11	1:A:286:ARG:HG3	1.74	0.52
1:D:148:MET:HE2	1:D:187:SER:HA	1.90	0.52
1:D:1:MET:HB3	2:D:2002:HOH:O	2.09	0.52
1:B:317:ILE:O	1:B:383:MET:HB2	2.10	0.52
1:B:400:TYR:HB2	1:B:482:PRO:HG3	1.92	0.52
1:C:148:MET:HE1	1:C:187:SER:HA	1.90	0.52
1:A:463:ARG:NH2	2:A:2119:HOH:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:GLN:HE21	1:A:307:ARG:NH2	2.04	0.51
1:A:400:TYR:HB2	1:A:482:PRO:HG3	1.92	0.51
1:B:150:HIS:O	1:B:151:TRP:HB2	2.10	0.51
1:A:80:LEU:HD12	1:A:80:LEU:N	2.25	0.51
1:C:280:MET:HE2	1:C:333:GLY:HA2	1.92	0.51
1:D:192:TRP:HA	1:D:253:VAL:CG1	2.39	0.51
1:B:328:LYS:CD	1:B:337:LEU:HD21	2.41	0.51
1:A:320:ASN:CG	1:A:387:GLU:HB2	2.31	0.51
1:C:150:HIS:O	1:C:151:TRP:HB2	2.10	0.51
1:A:184:ALA:HB2	1:A:245:ARG:HB3	1.93	0.51
1:D:328:LYS:CD	1:D:337:LEU:HD21	2.41	0.51
1:D:329:ARG:NH1	1:D:329:ARG:HG3	2.26	0.51
1:C:320:ASN:CG	1:C:387:GLU:HB2	2.31	0.50
1:C:400:TYR:HB2	1:C:482:PRO:HG3	1.92	0.50
1:C:328:LYS:CD	1:C:337:LEU:HD21	2.41	0.50
1:A:271:THR:HG21	1:A:273:LYS:HZ3	1.76	0.50
1:B:299:THR:HB	1:B:304:LYS:HE3	1.92	0.50
1:B:305:ILE:CG2	1:B:306:VAL:H	2.19	0.50
1:C:423:LEU:HD12	1:C:423:LEU:N	2.27	0.50
1:D:148:MET:CE	1:D:190:THR:HB	2.39	0.50
1:D:400:TYR:HB2	1:D:482:PRO:HG3	1.93	0.50
1:A:305:ILE:CG2	1:A:306:VAL:H	2.18	0.50
1:A:335:VAL:HG12	1:A:336:SER:O	2.12	0.50
1:A:328:LYS:CD	1:A:337:LEU:HD21	2.40	0.50
1:D:317:ILE:O	1:D:383:MET:HB2	2.12	0.50
1:B:103:GLN:OE1	1:B:300:ARG:HD3	2.11	0.50
1:C:299:THR:HB	1:C:304:LYS:HE3	1.94	0.50
1:C:80:LEU:N	1:C:80:LEU:HD12	2.26	0.50
1:D:320:ASN:CG	1:D:387:GLU:HB2	2.31	0.50
1:C:184:ALA:HB2	1:C:245:ARG:HB3	1.94	0.50
1:A:162:ARG:NH1	1:A:170:GLY:N	2.60	0.49
1:D:148:MET:HE1	1:D:187:SER:HA	1.93	0.49
1:D:94:ARG:HB3	1:D:94:ARG:NH1	2.26	0.49
1:C:138:LYS:HD2	1:C:197:LEU:O	2.12	0.49
1:C:286:ARG:HH11	1:C:286:ARG:HG3	1.77	0.49
1:A:219:LYS:HD3	1:B:47:LEU:HD23	1.94	0.49
1:B:320:ASN:CG	1:B:387:GLU:HB2	2.33	0.49
1:A:192:TRP:HA	1:A:253:VAL:CG1	2.40	0.49
1:B:53:PRO:HD2	1:B:54:GLU:OE2	2.13	0.49
1:A:329:ARG:HD3	1:A:333:GLY:O	2.13	0.49
1:C:317:ILE:O	1:C:383:MET:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:LYS:HD2	1:A:197:LEU:O	2.12	0.48
1:B:138:LYS:HD2	1:B:197:LEU:O	2.13	0.48
1:D:162:ARG:NH1	1:D:170:GLY:N	2.61	0.48
1:D:53:PRO:HD2	1:D:54:GLU:OE2	2.13	0.48
1:A:148:MET:HE2	1:A:187:SER:HA	1.95	0.48
1:A:317:ILE:O	1:A:383:MET:HB2	2.13	0.48
1:A:53:PRO:HD2	1:A:54:GLU:OE2	2.14	0.48
1:D:138:LYS:HD2	1:D:197:LEU:O	2.14	0.48
1:A:154:PRO:HG2	1:A:157:LEU:HD12	1.94	0.48
1:A:105:VAL:H	1:A:241:GLN:HE22	1.60	0.48
1:B:80:LEU:HD12	1:B:80:LEU:N	2.28	0.48
1:D:154:PRO:HG2	1:D:157:LEU:HD12	1.96	0.48
1:D:80:LEU:N	1:D:80:LEU:HD12	2.29	0.48
1:A:108:VAL:HG23	1:A:245:ARG:HG2	1.96	0.48
1:B:184:ALA:HB2	1:B:245:ARG:HB3	1.96	0.48
1:C:162:ARG:NH1	1:C:170:GLY:N	2.61	0.48
1:C:53:PRO:HD2	1:C:54:GLU:OE2	2.13	0.47
1:D:489:HIS:HB3	2:D:2115:HOH:O	2.14	0.47
1:A:94:ARG:HG2	1:A:95:PRO:CD	2.44	0.47
1:C:335:VAL:HG12	1:C:336:SER:O	2.14	0.47
1:D:83:GLU:HB2	1:D:86:ARG:HG3	1.96	0.47
1:A:305:ILE:CG2	1:A:306:VAL:N	2.75	0.47
1:A:96:GLN:OE1	1:A:96:GLN:N	2.42	0.47
1:A:423:LEU:N	1:A:423:LEU:HD12	2.30	0.47
1:C:150:HIS:O	1:C:152:PRO:HD3	2.15	0.47
1:B:148:MET:CE	1:B:190:THR:HB	2.41	0.47
1:B:271:THR:CG2	1:B:272:ASP:N	2.77	0.47
1:D:184:ALA:HB2	1:D:245:ARG:HB3	1.96	0.47
1:B:105:VAL:H	1:B:241:GLN:HE22	1.60	0.47
1:C:154:PRO:HG2	1:C:157:LEU:HD12	1.97	0.47
1:C:192:TRP:HA	1:C:253:VAL:CG1	2.40	0.47
1:D:108:VAL:HG23	1:D:245:ARG:HG2	1.96	0.47
1:C:94:ARG:CZ	1:C:94:ARG:HB3	2.45	0.47
1:D:150:HIS:O	1:D:152:PRO:HD3	2.15	0.47
1:A:271:THR:CG2	1:A:272:ASP:N	2.77	0.47
1:A:94:ARG:HH11	1:A:94:ARG:HB3	1.80	0.47
1:C:271:THR:CG2	1:C:272:ASP:N	2.76	0.47
1:D:241:GLN:HE21	1:D:307:ARG:NH1	2.12	0.47
1:B:162:ARG:NH1	1:B:170:GLY:N	2.62	0.47
1:A:241:GLN:HE21	1:A:307:ARG:NH1	2.11	0.46
1:C:241:GLN:HE21	1:C:307:ARG:NH1	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:ARG:HG2	1:A:95:PRO:HD2	1.97	0.46
1:B:192:TRP:HA	1:B:253:VAL:CG1	2.42	0.46
1:B:335:VAL:HG12	1:B:336:SER:O	2.14	0.46
1:D:298:ILE:HG12	1:D:299:THR:N	2.30	0.46
1:D:96:GLN:N	1:D:96:GLN:OE1	2.48	0.46
1:A:96:GLN:O	1:A:97:ASN:OD1	2.34	0.46
1:C:105:VAL:H	1:C:241:GLN:HE22	1.63	0.46
1:D:191:ALA:O	1:D:195:ASP:HB2	2.16	0.46
1:A:60:TRP:O	1:A:129:HIS:HE1	1.98	0.46
1:C:95:PRO:HB2	1:C:98:PHE:HB2	1.98	0.46
1:D:60:TRP:O	1:D:129:HIS:HE1	1.97	0.46
1:B:108:VAL:HG23	1:B:245:ARG:HG2	1.96	0.46
1:A:329:ARG:HG3	1:A:329:ARG:NH1	2.31	0.46
1:C:253:VAL:O	1:C:253:VAL:HG12	2.16	0.46
1:C:83:GLU:HB2	1:C:86:ARG:HG3	1.96	0.46
1:D:423:LEU:HD12	1:D:423:LEU:N	2.30	0.46
1:B:288:TRP:CG	1:B:289:PHE:N	2.84	0.46
1:A:237:TYR:CZ	1:A:300:ARG:HB3	2.51	0.46
1:B:154:PRO:HG2	1:B:157:LEU:HD12	1.98	0.46
1:B:241:GLN:HE21	1:B:307:ARG:NH1	2.12	0.46
1:B:276:GLU:O	1:B:280:MET:HG3	2.16	0.46
1:D:271:THR:CG2	1:D:272:ASP:N	2.78	0.46
1:D:271:THR:HG21	1:D:273:LYS:HZ2	1.79	0.46
1:B:60:TRP:O	1:B:129:HIS:HE1	1.99	0.45
1:B:83:GLU:HB2	1:B:86:ARG:HG3	1.98	0.45
1:C:60:TRP:O	1:C:129:HIS:HE1	1.98	0.45
1:D:303:GLU:CD	1:D:303:GLU:N	2.69	0.45
1:A:150:HIS:O	1:A:152:PRO:HD3	2.16	0.45
1:A:276:GLU:O	1:A:280:MET:HG3	2.16	0.45
1:B:307:ARG:HB3	1:B:309:ASP:OD1	2.16	0.45
1:D:237:TYR:CE1	1:D:300:ARG:HB3	2.51	0.45
1:A:300:ARG:HG2	1:A:300:ARG:HH11	1.81	0.45
1:C:98:PHE:CZ	1:C:181:TYR:HB2	2.51	0.45
1:D:300:ARG:HG2	1:D:300:ARG:HH11	1.82	0.45
1:A:138:LYS:HA	1:A:138:LYS:HE2	1.98	0.45
1:A:298:ILE:HG12	1:A:299:THR:N	2.31	0.45
1:A:94:ARG:CZ	1:A:94:ARG:HB3	2.47	0.45
1:B:138:LYS:HA	1:B:138:LYS:HE2	1.99	0.45
1:B:298:ILE:HG12	1:B:299:THR:N	2.32	0.45
1:D:105:VAL:H	1:D:241:GLN:HE22	1.62	0.45
1:B:150:HIS:O	1:B:152:PRO:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:423:LEU:N	1:B:423:LEU:HD12	2.31	0.45
1:B:329:ARG:HG3	1:B:329:ARG:HH11	1.82	0.45
1:C:237:TYR:CE1	1:C:300:ARG:HB3	2.52	0.45
1:C:298:ILE:HG12	1:C:299:THR:N	2.32	0.45
1:D:288:TRP:CG	1:D:289:PHE:N	2.84	0.45
1:D:335:VAL:HG12	1:D:336:SER:O	2.16	0.45
1:B:191:ALA:O	1:B:195:ASP:HB2	2.16	0.45
1:D:446:VAL:HG22	1:D:453:LEU:CD2	2.47	0.45
1:B:271:THR:HG21	1:B:273:LYS:HZ3	1.81	0.44
1:D:291:ASP:O	1:D:295:ARG:HB2	2.17	0.44
1:C:108:VAL:HG23	1:C:245:ARG:HG2	1.98	0.44
1:C:191:ALA:O	1:C:195:ASP:HB2	2.17	0.44
1:D:298:ILE:HG12	1:D:299:THR:H	1.83	0.44
1:A:162:ARG:HH12	1:A:170:GLY:N	2.16	0.44
1:C:300:ARG:O	1:C:300:ARG:HD2	2.17	0.44
1:D:276:GLU:O	1:D:280:MET:HG3	2.17	0.44
1:A:138:LYS:HE3	1:A:142:LEU:O	2.18	0.44
1:A:191:ALA:O	1:A:195:ASP:HB2	2.17	0.44
1:A:83:GLU:HB2	1:A:86:ARG:HG3	1.99	0.44
1:D:16:GLY:HA2	1:D:20:GLU:HG3	2.00	0.44
1:A:104:ASP:CA	1:A:241:GLN:HE22	2.24	0.44
1:C:245:ARG:NE	1:C:245:ARG:HA	2.33	0.44
1:B:474:GLU:H	1:B:474:GLU:CD	2.21	0.44
1:C:3:SER:HA	1:C:470:ALA:CB	2.48	0.44
1:D:138:LYS:HE3	1:D:142:LEU:O	2.18	0.44
1:D:1:MET:HG2	1:D:2:TYR:N	2.33	0.44
1:A:148:MET:CE	1:A:190:THR:HB	2.42	0.43
1:D:112:GLU:O	1:D:116:LYS:HG2	2.18	0.43
1:D:150:HIS:O	1:D:151:TRP:CB	2.66	0.43
1:A:3:SER:HA	1:A:470:ALA:CB	2.48	0.43
1:D:245:ARG:HA	1:D:245:ARG:NE	2.33	0.43
1:B:39:ASP:OD2	1:B:164:ARG:NH2	2.52	0.43
1:B:96:GLN:CG	1:B:97:ASN:N	2.79	0.43
1:C:104:ASP:CA	1:C:241:GLN:HE22	2.24	0.43
1:C:288:TRP:CG	1:C:289:PHE:N	2.86	0.43
1:C:307:ARG:HB3	1:C:309:ASP:OD1	2.18	0.43
1:D:3:SER:HA	1:D:470:ALA:CB	2.47	0.43
1:A:117:ARG:HH11	1:A:117:ARG:HB2	1.84	0.43
1:B:253:VAL:O	1:B:253:VAL:HG12	2.17	0.43
1:C:298:ILE:HG12	1:C:299:THR:H	1.84	0.43
1:C:276:GLU:O	1:C:280:MET:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HG2	1:C:2:TYR:N	2.33	0.43
1:A:332:LYS:HG3	1:A:333:GLY:N	2.27	0.43
1:A:446:VAL:HG22	1:A:453:LEU:CD2	2.49	0.43
1:C:148:MET:CE	1:C:190:THR:HB	2.44	0.43
1:C:332:LYS:HE3	1:C:332:LYS:HA	2.01	0.43
1:C:474:GLU:CD	1:C:474:GLU:H	2.20	0.43
1:D:307:ARG:HB3	1:D:309:ASP:OD1	2.19	0.43
1:A:112:GLU:O	1:A:116:LYS:HG2	2.19	0.43
1:A:288:TRP:CG	1:A:289:PHE:N	2.86	0.43
1:A:300:ARG:NH1	1:A:300:ARG:HG2	2.33	0.43
1:C:305:ILE:CG2	1:C:306:VAL:H	2.21	0.43
1:C:422:TYR:C	1:C:423:LEU:HD12	2.39	0.43
1:C:112:GLU:O	1:C:116:LYS:HG2	2.19	0.42
1:C:138:LYS:HE3	1:C:142:LEU:O	2.19	0.42
1:C:291:ASP:O	1:C:295:ARG:HB2	2.17	0.42
1:D:474:GLU:CD	1:D:474:GLU:H	2.21	0.42
1:A:298:ILE:HG12	1:A:299:THR:H	1.84	0.42
1:C:137:LEU:HD12	1:C:142:LEU:HD12	2.01	0.42
1:A:304:LYS:HD3	1:A:305:ILE:N	2.35	0.42
1:A:474:GLU:CD	1:A:474:GLU:H	2.21	0.42
1:B:138:LYS:HE3	1:B:142:LEU:O	2.19	0.42
1:C:117:ARG:HH11	1:C:117:ARG:HB2	1.84	0.42
1:A:253:VAL:HG12	1:A:253:VAL:O	2.18	0.42
1:D:39:ASP:OD2	1:D:164:ARG:NH2	2.52	0.42
1:D:422:TYR:C	1:D:423:LEU:HD12	2.40	0.42
1:A:150:HIS:O	1:A:151:TRP:CB	2.67	0.42
1:A:245:ARG:NE	1:A:245:ARG:HA	2.34	0.42
1:C:446:VAL:HG22	1:C:453:LEU:CD2	2.49	0.42
1:D:138:LYS:HE2	1:D:138:LYS:HA	2.01	0.42
1:B:298:ILE:HG12	1:B:299:THR:H	1.84	0.42
1:D:117:ARG:HH11	1:D:117:ARG:HB2	1.83	0.42
1:D:162:ARG:HH12	1:D:170:GLY:N	2.18	0.42
1:B:234:ARG:HH11	1:B:234:ARG:HG3	1.84	0.42
1:B:422:TYR:C	1:B:423:LEU:HD12	2.40	0.42
1:C:138:LYS:HA	1:C:138:LYS:HE2	2.02	0.42
1:C:94:ARG:HG2	1:C:95:PRO:HD2	2.02	0.42
1:A:303:GLU:OE1	1:A:305:ILE:HD11	2.20	0.42
1:A:422:TYR:C	1:A:423:LEU:HD12	2.40	0.42
1:B:76:LYS:CA	1:B:142:LEU:HD23	2.47	0.42
1:B:112:GLU:O	1:B:116:LYS:HG2	2.19	0.42
1:B:245:ARG:HA	1:B:245:ARG:NE	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:GLY:HA2	1:C:20:GLU:HG3	2.01	0.42
1:C:262:TYR:O	1:C:320:ASN:HB2	2.20	0.42
1:A:43:MET:HE1	2:A:2023:HOH:O	2.19	0.41
1:D:253:VAL:HG12	1:D:253:VAL:O	2.18	0.41
1:D:241:GLN:NE2	1:D:307:ARG:HH22	2.10	0.41
1:A:1:MET:HG2	1:A:2:TYR:N	2.34	0.41
1:A:16:GLY:HA2	1:A:20:GLU:HG3	2.02	0.41
1:D:234:ARG:HH11	1:D:234:ARG:HG3	1.86	0.41
1:D:349:VAL:CG1	1:D:353:GLY:HA2	2.50	0.41
1:A:241:GLN:NE2	1:A:307:ARG:HH22	2.12	0.41
1:D:139:SER:HA	2:D:2041:HOH:O	2.20	0.41
1:D:79:ARG:NH2	1:D:205:ASN:OD1	2.51	0.41
1:A:137:LEU:HD12	1:A:142:LEU:HD12	2.03	0.41
1:A:307:ARG:HB3	1:A:309:ASP:OD1	2.20	0.41
1:B:11:GLY:HA3	1:B:77:ILE:O	2.20	0.41
1:B:34:TYR:CZ	1:B:38:HIS:CE1	3.09	0.41
1:B:463:ARG:HD2	2:B:2094:HOH:O	2.20	0.41
1:B:1:MET:HG2	1:B:2:TYR:N	2.36	0.41
1:C:162:ARG:HH12	1:C:170:GLY:N	2.18	0.41
1:C:189:TYR:CZ	1:C:193:LYS:HD2	2.56	0.41
1:D:300:ARG:NH1	1:D:300:ARG:HG2	2.35	0.41
1:A:291:ASP:O	1:A:295:ARG:HB2	2.20	0.41
1:B:3:SER:HA	1:B:470:ALA:CB	2.48	0.41
1:A:228:SER:HA	1:B:41:GLU:OE2	2.20	0.41
1:D:349:VAL:HG13	1:D:353:GLY:HA2	2.03	0.41
1:D:60:TRP:O	1:D:129:HIS:CE1	2.73	0.41
1:A:39:ASP:OD2	1:A:164:ARG:NH2	2.54	0.41
1:A:234:ARG:HG3	1:A:234:ARG:HH11	1.86	0.41
1:B:5:PRO:HD3	2:B:2002:HOH:O	2.19	0.41
1:D:463:ARG:HD2	2:D:2109:HOH:O	2.21	0.41
1:A:17:PHE:HB2	1:A:152:PRO:HG2	2.03	0.41
1:D:88:PHE:CE1	1:D:118:LEU:HD22	2.56	0.41
1:D:151:TRP:CD1	1:D:151:TRP:N	2.89	0.41
1:B:88:PHE:CE1	1:B:118:LEU:HD22	2.56	0.41
1:B:17:PHE:HB2	1:B:152:PRO:HG2	2.03	0.41
1:B:291:ASP:O	1:B:295:ARG:HB2	2.21	0.41
1:C:52:LEU:HA	1:C:53:PRO:HD3	1.92	0.41
1:D:189:TYR:CZ	1:D:193:LYS:HD2	2.56	0.41
1:B:209:VAL:HG13	1:B:213:LEU:HD12	2.03	0.40
1:C:17:PHE:HB2	1:C:152:PRO:HG2	2.03	0.40
1:C:148:MET:HB2	1:C:203:THR:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ARG:HH11	1:C:234:ARG:HG3	1.85	0.40
1:D:26:SER:O	1:D:86:ARG:NH2	2.51	0.40
1:B:52:LEU:HB3	1:B:54:GLU:OE2	2.20	0.40
1:A:90:ASN:HA	1:A:91:PRO:HD3	1.93	0.40
1:B:131:ARG:O	1:B:135:LYS:HG3	2.21	0.40
1:B:189:TYR:CZ	1:B:193:LYS:HD2	2.56	0.40
1:B:162:ARG:HH12	1:B:170:GLY:N	2.20	0.40
1:B:271:THR:CG2	1:B:273:LYS:HG2	2.51	0.40
1:B:262:TYR:O	1:B:320:ASN:HB2	2.22	0.40
1:C:398:ARG:HD2	1:C:458:SER:OG	2.21	0.40
1:D:52:LEU:HA	1:D:53:PRO:HD3	1.91	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	487/489 (100%)	463 (95%)	21 (4%)	3 (1%)	28	46
1	B	487/489 (100%)	463 (95%)	20 (4%)	4 (1%)	22	38
1	C	487/489 (100%)	467 (96%)	18 (4%)	2 (0%)	38	57
1	D	487/489 (100%)	465 (96%)	19 (4%)	3 (1%)	28	46
All	All	1948/1956 (100%)	1858 (95%)	78 (4%)	12 (1%)	28	46

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	TRP
1	A	331	GLY
1	B	151	TRP
1	C	151	TRP

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Mol	Chain	Res	Type
1	D	151	TRP
1	B	331	GLY
1	B	332	LYS
1	A	426	SER
1	B	426	SER
1	C	426	SER
1	D	426	SER
1	D	333	GLY

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	421/421 (100%)	405 (96%)	16 (4%)	38	62
1	B	421/421 (100%)	405 (96%)	16 (4%)	38	62
1	C	421/421 (100%)	405 (96%)	16 (4%)	38	62
1	D	421/421 (100%)	403 (96%)	18 (4%)	33	56
All	All	1684/1684 (100%)	1618 (96%)	66 (4%)	37	61

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	ARG
1	A	96	GLN
1	A	118	LEU
1	A	245	ARG
1	A	272	ASP
1	A	299	THR
1	A	300	ARG
1	A	304	LYS
1	A	324	ARG
1	A	329	ARG
1	A	349	VAL
1	A	359	PHE
1	A	427	LEU

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Mol	Chain	Res	Type
1	A	449	ASN
1	A	467	THR
1	A	474	GLU
1	B	79	ARG
1	B	118	LEU
1	B	245	ARG
1	B	272	ASP
1	B	299	THR
1	B	300	ARG
1	B	304	LYS
1	B	324	ARG
1	B	329	ARG
1	B	332	LYS
1	B	349	VAL
1	B	359	PHE
1	B	427	LEU
1	B	449	ASN
1	B	467	THR
1	B	474	GLU
1	C	79	ARG
1	C	94	ARG
1	C	118	LEU
1	C	245	ARG
1	C	272	ASP
1	C	299	THR
1	C	300	ARG
1	C	304	LYS
1	C	324	ARG
1	C	332	LYS
1	C	349	VAL
1	C	359	PHE
1	C	427	LEU
1	C	449	ASN
1	C	467	THR
1	C	474	GLU
1	D	79	ARG
1	D	80	LEU
1	D	96	GLN
1	D	97	ASN
1	D	118	LEU
1	D	245	ARG
1	D	272	ASP

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Mol	Chain	Res	Type
1	D	299	THR
1	D	300	ARG
1	D	324	ARG
1	D	329	ARG
1	D	332	LYS
1	D	349	VAL
1	D	359	PHE
1	D	427	LEU
1	D	449	ASN
1	D	467	THR
1	D	474	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	128	ASN
1	A	129	HIS
1	A	241	GLN
1	A	264	ASN
1	A	342	HIS
1	A	410	HIS
1	A	430	ASN
1	A	479	ASN
1	A	489	HIS
1	B	18	GLN
1	B	55	ASN
1	B	96	GLN
1	B	128	ASN
1	B	129	HIS
1	B	146	GLN
1	B	241	GLN
1	B	264	ASN
1	B	342	HIS
1	B	410	HIS
1	B	430	ASN
1	B	479	ASN
1	C	18	GLN
1	C	55	ASN
1	C	128	ASN
1	C	129	HIS
1	C	146	GLN

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Mol	Chain	Res	Type
1	C	241	GLN
1	C	264	ASN
1	C	342	HIS
1	C	410	HIS
1	C	430	ASN
1	C	479	ASN
1	D	18	GLN
1	D	97	ASN
1	D	128	ASN
1	D	129	HIS
1	D	241	GLN
1	D	264	ASN
1	D	342	HIS
1	D	410	HIS
1	D	430	ASN
1	D	479	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	489/489 (100%)	0.29	34 (6%)	17 18	19, 28, 54, 76	0
1	B	489/489 (100%)	0.30	37 (7%)	15 15	19, 28, 56, 78	0
1	C	489/489 (100%)	0.27	40 (8%)	12 13	19, 29, 56, 84	0
1	D	489/489 (100%)	0.25	22 (4%)	34 37	18, 28, 53, 72	0
All	All	1956/1956 (100%)	0.28	133 (6%)	18 19	18, 29, 55, 84	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	302	ASN	7.5
1	D	141	GLY	7.4
1	B	332	LYS	6.7
1	B	97	ASN	6.7
1	B	303	GLU	6.4
1	C	301	GLY	6.2
1	A	97	ASN	6.0
1	D	302	ASN	5.9
1	C	299	THR	5.7
1	D	1	MET	5.7
1	C	303	GLU	5.6
1	B	301	GLY	5.4
1	C	113	ASN	5.4
1	B	96	GLN	5.2
1	B	302	ASN	5.2
1	C	97	ASN	5.0
1	D	97	ASN	5.0
1	B	333	GLY	4.8
1	A	96	GLN	4.8
1	C	272	ASP	4.8
1	C	96	GLN	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	331	GLY	4.4
1	C	273	LYS	4.4
1	C	305	ILE	4.3
1	D	303	GLU	4.2
1	B	305	ILE	4.2
1	C	304	LYS	4.1
1	B	116	LYS	3.9
1	C	300	ARG	3.9
1	B	329	ARG	3.9
1	A	330	THR	3.9
1	B	304	LYS	3.8
1	B	273	LYS	3.8
1	B	271	THR	3.8
1	A	271	THR	3.8
1	A	94	ARG	3.7
1	A	1	MET	3.7
1	B	98	PHE	3.7
1	A	273	LYS	3.6
1	D	304	LYS	3.5
1	C	116	LYS	3.5
1	A	414	ASN	3.4
1	A	82	SER	3.4
1	A	272	ASP	3.4
1	B	99	ASP	3.4
1	C	112	GLU	3.3
1	C	329	ARG	3.3
1	C	99	ASP	3.3
1	D	96	GLN	3.3
1	A	117	ARG	3.2
1	D	305	ILE	3.1
1	D	117	ARG	3.0
1	A	102	LYS	3.0
1	A	332	LYS	3.0
1	A	331	GLY	3.0
1	C	100	GLU	3.0
1	B	299	THR	2.9
1	B	113	ASN	2.9
1	A	183	PHE	2.9
1	B	203	THR	2.8
1	D	301	GLY	2.8
1	A	101	SER	2.8
1	A	302	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	335	VAL	2.7
1	C	128	ASN	2.7
1	B	100	GLU	2.7
1	B	272	ASP	2.7
1	C	253	VAL	2.7
1	A	304	LYS	2.7
1	B	6	ASN	2.7
1	D	230	GLU	2.6
1	C	101	SER	2.6
1	A	305	ILE	2.6
1	C	333	GLY	2.6
1	C	252	SER	2.6
1	B	300	ARG	2.6
1	D	94	ARG	2.6
1	D	300	ARG	2.6
1	B	328	LYS	2.6
1	A	328	LYS	2.5
1	A	329	ARG	2.5
1	C	489	HIS	2.5
1	C	426	SER	2.5
1	B	274	ASP	2.5
1	C	169	THR	2.5
1	C	109	GLU	2.5
1	C	117	ARG	2.5
1	C	306	VAL	2.5
1	C	332	LYS	2.4
1	C	68	ASN	2.4
1	C	271	THR	2.4
1	D	426	SER	2.4
1	A	186	PHE	2.4
1	C	280	MET	2.4
1	A	109	GLU	2.4
1	C	6	ASN	2.3
1	A	426	SER	2.3
1	C	94	ARG	2.3
1	A	84	TRP	2.3
1	B	94	ARG	2.3
1	A	275	MET	2.3
1	A	489	HIS	2.3
1	C	93	PRO	2.3
1	C	98	PHE	2.3
1	B	489	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	139	SER	2.2
1	B	109	GLU	2.2
1	D	186	PHE	2.2
1	B	204	MET	2.2
1	C	102	LYS	2.2
1	B	426	SER	2.2
1	B	1	MET	2.1
1	B	330	THR	2.1
1	A	260	ILE	2.1
1	C	152	PRO	2.1
1	B	101	SER	2.1
1	D	449	ASN	2.1
1	D	2	TYR	2.1
1	D	329	ARG	2.1
1	A	274	ASP	2.1
1	A	276	GLU	2.1
1	B	2	TYR	2.1
1	A	6	ASN	2.1
1	C	255	LYS	2.1
1	B	148	MET	2.0
1	D	81	ASN	2.0
1	A	162	ARG	2.0
1	D	140	ARG	2.0
1	B	335	VAL	2.0
1	D	128	ASN	2.0
1	B	196	ASP	2.0
1	A	93	PRO	2.0
1	A	153	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.