



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2021 – 03:55 PM EST

PDB ID : 1XRH
Title : Crystal Structure of Ureidoglycolate Dehydrogenase from Escherichia Coli
Authors : Rajashankar, K.R.; Kniewel, R.; Lima, C.D.; Burley, S.K.; New York SGX
Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2004-10-14
Resolution : 2.25 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.16
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.16

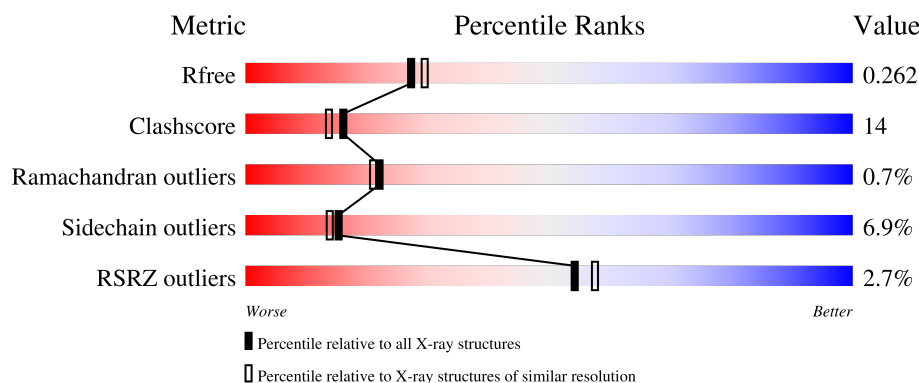
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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	351	<div> <div>3%</div> <div>67%</div> <div>26%</div> <div>5%</div> <div>.</div> </div>
1	B	351	<div> <div>2%</div> <div>71%</div> <div>24%</div> <div>.</div> <div>.</div> </div>
1	C	351	<div> <div>3%</div> <div>69%</div> <div>27%</div> <div>.</div> <div>.</div> </div>
1	D	351	<div> <div>%</div> <div>69%</div> <div>26%</div> <div>.</div> <div>.</div> </div>
1	E	351	<div> <div>5%</div> <div>63%</div> <div>30%</div> <div>.</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	351	<div><div>%</div><div><div></div><div>67%</div><div>26%</div><div></div><div></div></div></div>
1	G	351	<div><div>3%</div><div><div></div><div>71%</div><div>22%</div><div></div><div></div></div></div>
1	H	351	<div><div>2%</div><div><div></div><div>75%</div><div>20%</div><div></div><div></div></div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 21480 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 Ureidoglycolate Dehydrogenase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	Se	0	0	0
			2616	1647	457	497	3	12			
1	B	343	Total	C	N	O	S	Se	0	0	0
			2616	1647	457	497	3	12			
1	C	344	Total	C	N	O	S	Se	0	0	0
			2622	1650	458	499	3	12			
1	D	342	Total	C	N	O	S	Se	0	0	0
			2607	1642	456	494	3	12			
1	E	343	Total	C	N	O	S	Se	0	0	0
			2616	1647	457	497	3	12			
1	F	339	Total	C	N	O	S	Se	0	0	0
			2582	1626	453	488	3	12			
1	G	341	Total	C	N	O	S	Se	0	0	0
			2595	1633	455	492	3	12			
1	H	339	Total	C	N	O	S	Se	0	0	0
			2582	1626	453	488	3	12			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	cloning artifact	UNP P77555
A	2	SER	-	cloning artifact	UNP P77555
A	3	SER	MET	cloning artifact	UNP P77555
A	94	MSE	MET	modified residue	UNP P77555
A	96	MSE	MET	modified residue	UNP P77555
A	116	MSE	MET	modified residue	UNP P77555
A	139	MSE	MET	modified residue	UNP P77555
A	145	MSE	MET	modified residue	UNP P77555
A	177	MSE	MET	modified residue	UNP P77555
A	195	MSE	MET	modified residue	UNP P77555
A	231	MSE	MET	modified residue	UNP P77555
A	232	MSE	MET	modified residue	UNP P77555
A	233	MSE	MET	modified residue	UNP P77555

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Chain	Residue	Modelled	Actual	Comment	Reference
A	253	MSE	MET	modified residue	UNP P77555
A	289	MSE	MET	modified residue	UNP P77555
B	1	SER	-	cloning artifact	UNP P77555
B	2	SER	-	cloning artifact	UNP P77555
B	3	SER	MET	cloning artifact	UNP P77555
B	94	MSE	MET	modified residue	UNP P77555
B	96	MSE	MET	modified residue	UNP P77555
B	116	MSE	MET	modified residue	UNP P77555
B	139	MSE	MET	modified residue	UNP P77555
B	145	MSE	MET	modified residue	UNP P77555
B	177	MSE	MET	modified residue	UNP P77555
B	195	MSE	MET	modified residue	UNP P77555
B	231	MSE	MET	modified residue	UNP P77555
B	232	MSE	MET	modified residue	UNP P77555
B	233	MSE	MET	modified residue	UNP P77555
B	253	MSE	MET	modified residue	UNP P77555
B	289	MSE	MET	modified residue	UNP P77555
C	1	SER	-	cloning artifact	UNP P77555
C	2	SER	-	cloning artifact	UNP P77555
C	3	SER	MET	cloning artifact	UNP P77555
C	94	MSE	MET	modified residue	UNP P77555
C	96	MSE	MET	modified residue	UNP P77555
C	116	MSE	MET	modified residue	UNP P77555
C	139	MSE	MET	modified residue	UNP P77555
C	145	MSE	MET	modified residue	UNP P77555
C	177	MSE	MET	modified residue	UNP P77555
C	195	MSE	MET	modified residue	UNP P77555
C	231	MSE	MET	modified residue	UNP P77555
C	232	MSE	MET	modified residue	UNP P77555
C	233	MSE	MET	modified residue	UNP P77555
C	253	MSE	MET	modified residue	UNP P77555
C	289	MSE	MET	modified residue	UNP P77555
D	1	SER	-	cloning artifact	UNP P77555
D	2	SER	-	cloning artifact	UNP P77555
D	3	SER	MET	cloning artifact	UNP P77555
D	94	MSE	MET	modified residue	UNP P77555
D	96	MSE	MET	modified residue	UNP P77555
D	116	MSE	MET	modified residue	UNP P77555
D	139	MSE	MET	modified residue	UNP P77555
D	145	MSE	MET	modified residue	UNP P77555
D	177	MSE	MET	modified residue	UNP P77555
D	195	MSE	MET	modified residue	UNP P77555

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Chain	Residue	Modelled	Actual	Comment	Reference
D	231	MSE	MET	modified residue	UNP P77555
D	232	MSE	MET	modified residue	UNP P77555
D	233	MSE	MET	modified residue	UNP P77555
D	253	MSE	MET	modified residue	UNP P77555
D	289	MSE	MET	modified residue	UNP P77555
E	1	SER	-	cloning artifact	UNP P77555
E	2	SER	-	cloning artifact	UNP P77555
E	3	SER	MET	cloning artifact	UNP P77555
E	94	MSE	MET	modified residue	UNP P77555
E	96	MSE	MET	modified residue	UNP P77555
E	116	MSE	MET	modified residue	UNP P77555
E	139	MSE	MET	modified residue	UNP P77555
E	145	MSE	MET	modified residue	UNP P77555
E	177	MSE	MET	modified residue	UNP P77555
E	195	MSE	MET	modified residue	UNP P77555
E	231	MSE	MET	modified residue	UNP P77555
E	232	MSE	MET	modified residue	UNP P77555
E	233	MSE	MET	modified residue	UNP P77555
E	253	MSE	MET	modified residue	UNP P77555
E	289	MSE	MET	modified residue	UNP P77555
F	1	SER	-	cloning artifact	UNP P77555
F	2	SER	-	cloning artifact	UNP P77555
F	3	SER	MET	cloning artifact	UNP P77555
F	94	MSE	MET	modified residue	UNP P77555
F	96	MSE	MET	modified residue	UNP P77555
F	116	MSE	MET	modified residue	UNP P77555
F	139	MSE	MET	modified residue	UNP P77555
F	145	MSE	MET	modified residue	UNP P77555
F	177	MSE	MET	modified residue	UNP P77555
F	195	MSE	MET	modified residue	UNP P77555
F	231	MSE	MET	modified residue	UNP P77555
F	232	MSE	MET	modified residue	UNP P77555
F	233	MSE	MET	modified residue	UNP P77555
F	253	MSE	MET	modified residue	UNP P77555
F	289	MSE	MET	modified residue	UNP P77555
G	1	SER	-	cloning artifact	UNP P77555
G	2	SER	-	cloning artifact	UNP P77555
G	3	SER	MET	cloning artifact	UNP P77555
G	94	MSE	MET	modified residue	UNP P77555
G	96	MSE	MET	modified residue	UNP P77555
G	116	MSE	MET	modified residue	UNP P77555
G	139	MSE	MET	modified residue	UNP P77555

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Chain	Residue	Modelled	Actual	Comment	Reference
G	145	MSE	MET	modified residue	UNP P77555
G	177	MSE	MET	modified residue	UNP P77555
G	195	MSE	MET	modified residue	UNP P77555
G	231	MSE	MET	modified residue	UNP P77555
G	232	MSE	MET	modified residue	UNP P77555
G	233	MSE	MET	modified residue	UNP P77555
G	253	MSE	MET	modified residue	UNP P77555
G	289	MSE	MET	modified residue	UNP P77555
H	1	SER	-	cloning artifact	UNP P77555
H	2	SER	-	cloning artifact	UNP P77555
H	3	SER	MET	cloning artifact	UNP P77555
H	94	MSE	MET	modified residue	UNP P77555
H	96	MSE	MET	modified residue	UNP P77555
H	116	MSE	MET	modified residue	UNP P77555
H	139	MSE	MET	modified residue	UNP P77555
H	145	MSE	MET	modified residue	UNP P77555
H	177	MSE	MET	modified residue	UNP P77555
H	195	MSE	MET	modified residue	UNP P77555
H	231	MSE	MET	modified residue	UNP P77555
H	232	MSE	MET	modified residue	UNP P77555
H	233	MSE	MET	modified residue	UNP P77555
H	253	MSE	MET	modified residue	UNP P77555
H	289	MSE	MET	modified residue	UNP P77555

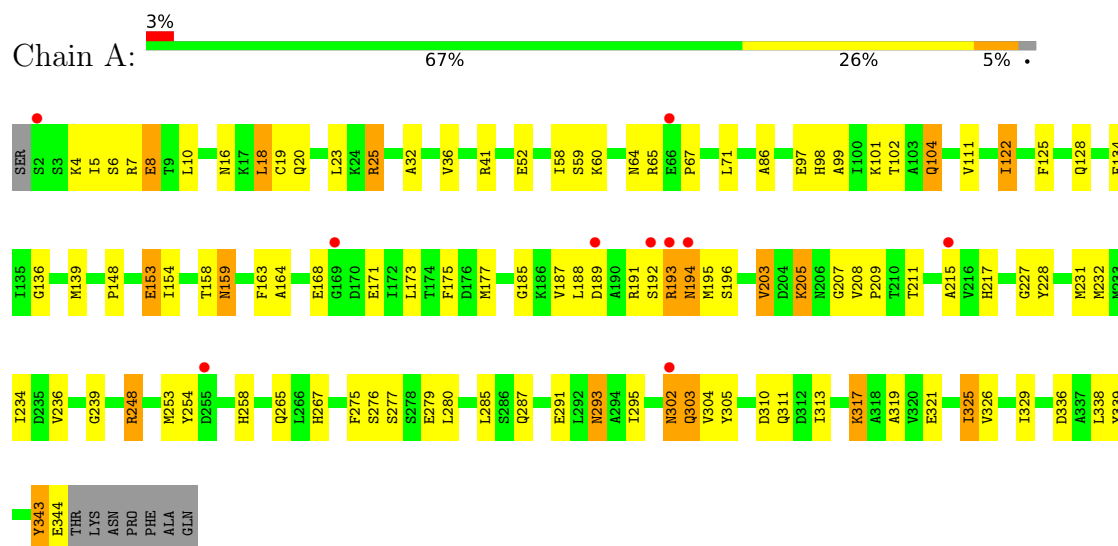
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	58	Total O 58 58	0	0
2	B	102	Total O 102 102	0	0
2	C	77	Total O 77 77	0	0
2	D	113	Total O 113 113	0	0
2	E	61	Total O 61 61	0	0
2	F	70	Total O 70 70	0	0
2	G	69	Total O 69 69	0	0
2	H	94	Total O 94 94	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.

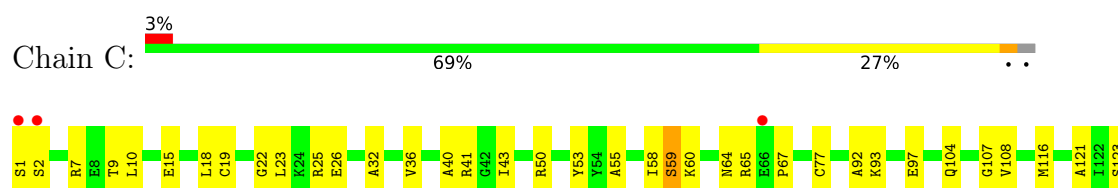
• Molecule 1: Ureidoglycolate Dehydrogenase

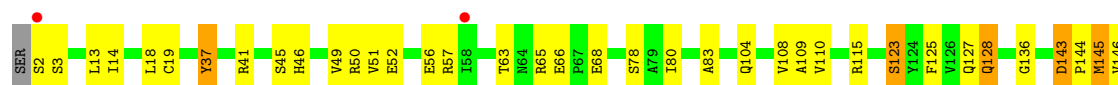


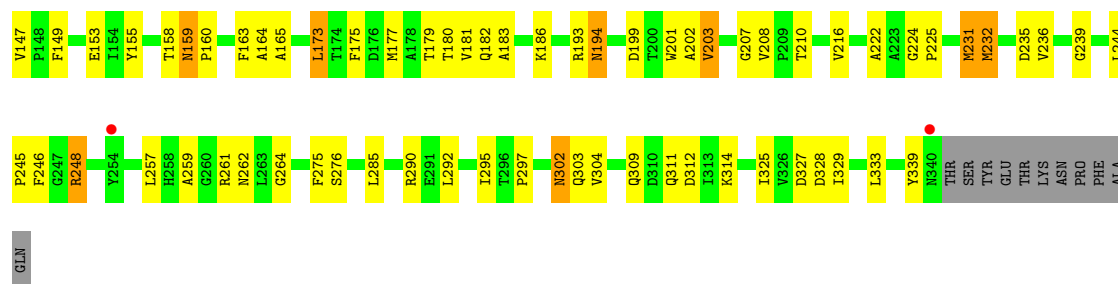
• Molecule 1: Ureidoglycolate Dehydrogenase



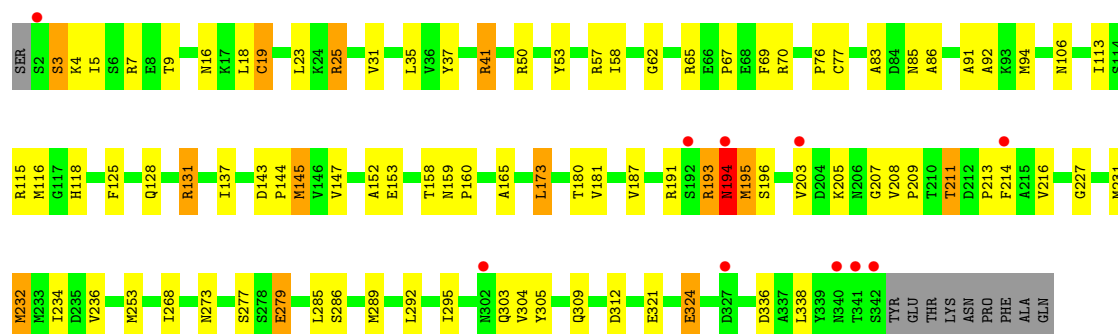
• Molecule 1: Ureidoglycolate Dehydrogenase



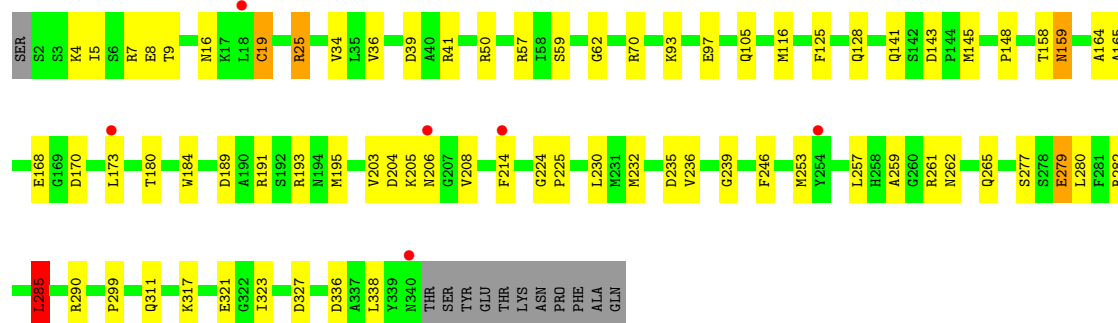
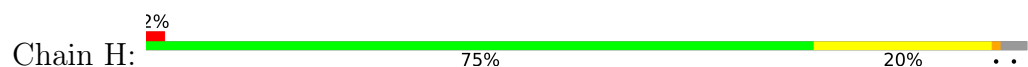




- Molecule 1: Ureidoglycolate Dehydrogenase



- Molecule 1: Ureidoglycolate Dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	104.72Å 129.92Å 106.47Å 90.00° 95.77° 90.00°	Depositor
Resolution (Å)	19.86 – 2.25 19.85 – 2.25	Depositor EDS
% Data completeness (in resolution range)	75.6 (19.86-2.25) 90.0 (19.85-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.26Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.192 , 0.250 0.206 , 0.262	Depositor DCC
R_{free} test set	9652 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	21480	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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	0.80	0/2660	0.83	1/3587 (0.0%)
1	B	0.88	1/2660 (0.0%)	0.90	1/3587 (0.0%)
1	C	0.82	0/2666	0.88	1/3595 (0.0%)
1	D	0.85	1/2651 (0.0%)	0.91	1/3575 (0.0%)
1	E	0.85	0/2660	0.86	2/3587 (0.1%)
1	F	0.83	0/2625	0.87	2/3539 (0.1%)
1	G	0.83	1/2638 (0.0%)	0.83	1/3557 (0.0%)
1	H	0.83	2/2625 (0.1%)	0.88	2/3539 (0.1%)
All	All	0.84	5/21185 (0.0%)	0.87	11/28566 (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
1	A	0	1
1	B	0	2
1	C	0	2
1	G	0	1
All	All	0	6

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	19	CYS	CB-SG	-7.29	1.69	1.82
1	H	168	GLU	CG-CD	6.58	1.61	1.51
1	B	19	CYS	CB-SG	-6.14	1.71	1.82
1	D	19	CYS	CB-SG	-5.68	1.72	1.81
1	H	19	CYS	CB-SG	-5.00	1.73	1.81

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	231	MSE	CG-SE-CE	-6.16	85.34	98.90
1	E	39	ASP	CB-CG-OD1	5.69	123.42	118.30
1	B	253	MSE	CB-CG-SE	-5.58	95.95	112.70
1	F	143	ASP	CB-CG-OD2	5.55	123.29	118.30
1	C	232	MSE	CG-SE-CE	5.47	110.94	98.90
1	G	41	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	A	122	ILE	CG1-CB-CG2	-5.33	99.67	111.40
1	E	212	ASP	CB-CG-OD2	5.30	123.07	118.30
1	H	282	ARG	NE-CZ-NH1	-5.25	117.68	120.30
1	D	50	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	H	285	LEU	CA-CB-CG	-5.03	103.73	115.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	343	TYR	Sidechain
1	B	228	TYR	Sidechain
1	B	343	TYR	Sidechain
1	C	228	TYR	Sidechain
1	C	330	TYR	Sidechain
1	G	53	TYR	Sidechain

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	2616	0	2559	89	0
1	B	2616	0	2559	86	0
1	C	2622	0	2567	76	0
1	D	2607	0	2553	74	0
1	E	2616	0	2559	109	0
1	F	2582	0	2532	79	0
1	G	2595	0	2544	87	0
1	H	2582	0	2532	53	0
2	A	58	0	0	0	0
2	B	102	0	0	5	0
2	C	77	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	113	0	0	4	0
2	E	61	0	0	7	0
2	F	70	0	0	1	0
2	G	69	0	0	7	0
2	H	94	0	0	3	0
All	All	21480	0	20405	597	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 (597) 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:E:50:ARG:HH21	1:E:253:MSE:HE1	1.09	1.15
1:G:232:MSE:HE2	1:G:236:VAL:HG21	1.27	1.14
1:A:153:GLU:HG3	1:B:295:ILE:HG23	1.34	1.10
1:A:232:MSE:HE3	1:B:173:LEU:HG	1.31	1.09
1:C:232:MSE:HE3	1:D:173:LEU:HD13	1.34	1.08
1:B:104:GLN:HG2	1:F:104:GLN:HG2	1.30	1.08
1:D:232:MSE:HE2	1:D:236:VAL:HG21	1.38	1.06
1:G:113:ILE:HG21	1:G:116:MSE:HE3	1.31	1.06
1:C:232:MSE:HE2	1:C:236:VAL:HG21	1.07	1.06
1:F:232:MSE:HE2	1:F:236:VAL:HG21	1.10	1.05
1:A:173:LEU:HD23	1:B:232:MSE:HE3	1.37	1.05
1:C:173:LEU:HD23	1:D:232:MSE:HE3	1.36	1.04
1:G:232:MSE:HE2	1:G:236:VAL:CG2	1.88	1.03
1:F:232:MSE:HE2	1:F:236:VAL:CG2	1.89	1.02
1:G:232:MSE:HE3	1:H:173:LEU:HD13	1.39	0.99
1:G:232:MSE:CE	1:G:236:VAL:HG21	1.92	0.98
1:D:232:MSE:HE2	1:D:236:VAL:CG2	1.95	0.96
1:F:41:ARG:NH1	1:F:311:GLN:HE21	1.65	0.94
1:C:232:MSE:HE2	1:C:236:VAL:CG2	1.97	0.93
1:C:205:LYS:HD3	1:C:217:HIS:HB2	1.51	0.93
1:E:48:ALA:O	1:E:51:VAL:HG12	1.69	0.91
1:F:232:MSE:CE	1:F:236:VAL:HG21	1.99	0.89
1:A:23:LEU:HG	1:A:58:ILE:HD13	1.54	0.89
1:G:196:SER:HB2	1:G:211:THR:HG23	1.55	0.88
1:E:303:GLN:HG2	1:E:304:VAL:H	1.35	0.88
1:A:173:LEU:CD2	1:B:232:MSE:HE3	2.04	0.87
1:F:41:ARG:HH12	1:F:311:GLN:HE21	1.22	0.87
1:G:173:LEU:CD2	1:H:232:MSE:HE3	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:196:SER:HB2	1:E:211:THR:HG22	1.57	0.87
1:G:113:ILE:CG2	1:G:116:MSE:HE3	2.06	0.86
1:A:177:MSE:CE	1:B:230:LEU:HG	2.06	0.85
1:C:232:MSE:HE3	1:D:173:LEU:CD1	2.06	0.85
1:E:50:ARG:NH2	1:E:253:MSE:HE1	1.91	0.85
1:B:145:MSE:HG3	2:B:444:HOH:O	1.79	0.83
1:D:41:ARG:HG3	1:D:311:GLN:HB3	1.58	0.83
1:E:227:GLY:O	1:E:231:MSE:HG3	1.77	0.83
1:G:277:SER:OG	1:G:279:GLU:HG2	1.79	0.82
1:D:232:MSE:CE	1:D:236:VAL:HG21	2.09	0.82
1:A:41:ARG:HE	1:A:311:GLN:HE21	1.26	0.81
1:B:232:MSE:HE2	1:B:236:VAL:HG21	1.61	0.80
1:E:148:PRO:HG2	1:F:295:ILE:HD13	1.64	0.80
1:F:165:ALA:HB3	1:F:285:LEU:HD21	1.63	0.80
1:C:232:MSE:CE	1:C:236:VAL:HG21	2.02	0.80
1:E:303:GLN:HG2	2:E:376:HOH:O	1.80	0.79
1:A:177:MSE:HE1	1:B:230:LEU:HG	1.64	0.79
1:A:227:GLY:O	1:A:231:MSE:HG3	1.83	0.79
1:A:232:MSE:CE	1:B:173:LEU:HG	2.11	0.78
1:B:232:MSE:HE2	1:B:236:VAL:CG2	2.12	0.78
1:C:286:SER:HA	1:C:289:MSE:HE3	1.67	0.77
1:E:290:ARG:O	1:E:293:ASN:HB2	1.86	0.76
1:F:41:ARG:NH1	1:F:311:GLN:NE2	2.32	0.76
1:G:113:ILE:HG21	1:G:116:MSE:CE	2.15	0.76
1:G:144:PRO:O	1:G:145:MSE:HG2	1.86	0.75
1:E:145:MSE:HG2	2:E:409:HOH:O	1.86	0.75
1:F:292:LEU:HA	1:F:295:ILE:HD12	1.69	0.75
1:A:104:GLN:HG2	1:A:134:PHE:HZ	1.52	0.75
1:A:205:LYS:HE2	1:A:217:HIS:HB2	1.68	0.74
1:H:205:LYS:HB3	1:H:205:LYS:NZ	2.02	0.73
1:C:60:LYS:HB3	1:C:258:HIS:CE1	2.24	0.73
1:E:197:ILE:O	1:E:211:THR:HG23	1.89	0.72
1:C:116:MSE:HE1	1:C:265:GLN:OE1	1.89	0.72
1:A:185:GLY:HA2	1:A:188:LEU:HD12	1.71	0.72
1:A:313:ILE:O	1:A:317:LYS:HG2	1.90	0.72
1:A:4:LYS:NZ	1:A:321:GLU:HB3	2.05	0.72
1:C:41:ARG:NH1	1:C:311:GLN:NE2	2.38	0.72
1:D:7:ARG:HG2	1:D:323:ILE:HD11	1.72	0.71
1:E:232:MSE:HE3	1:F:173:LEU:CD2	2.20	0.71
1:B:189:ASP:HB3	1:B:193:ARG:HH12	1.53	0.71
1:D:131:ARG:HD3	1:H:170:ASP:OD2	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:GLN:HE21	1:C:183:ALA:H	1.39	0.70
1:G:173:LEU:HD23	1:H:232:MSE:HE3	1.73	0.70
1:A:64:ASN:ND2	1:A:67:PRO:HA	2.06	0.70
1:H:277:SER:OG	1:H:279:GLU:HG2	1.90	0.70
1:G:152:ALA:O	2:G:378:HOH:O	2.10	0.69
1:G:158:THR:HG22	1:G:180:THR:HG21	1.74	0.69
1:A:104:GLN:HG2	1:A:134:PHE:CZ	2.27	0.69
1:B:232:MSE:CE	1:B:236:VAL:HG21	2.23	0.69
1:A:173:LEU:HD23	1:B:232:MSE:CE	2.16	0.69
1:F:41:ARG:HH12	1:F:311:GLN:NE2	1.90	0.69
1:C:173:LEU:CD2	1:D:232:MSE:HE3	2.20	0.69
1:E:193:ARG:HG3	1:E:193:ARG:HH11	1.59	0.68
1:A:41:ARG:HE	1:A:311:GLN:NE2	1.91	0.68
1:B:193:ARG:O	1:B:195:MSE:N	2.27	0.68
1:G:91:ALA:HB3	1:G:116:MSE:HE2	1.75	0.68
1:E:228:TYR:HA	1:E:231:MSE:HE2	1.76	0.68
1:D:145:MSE:HE3	1:D:219:LEU:HD12	1.75	0.67
1:G:279:GLU:CD	1:G:279:GLU:H	1.97	0.67
1:C:50:ARG:NH1	1:C:253:MSE:HE1	2.09	0.67
1:A:16:ASN:OD1	1:A:25:ARG:NH2	2.27	0.67
1:D:145:MSE:HE2	1:D:158:THR:HG23	1.76	0.67
1:E:327:ASP:O	1:E:331:GLN:HG3	1.93	0.67
1:E:7:ARG:HG3	1:E:36:VAL:HG11	1.76	0.67
1:F:165:ALA:CB	1:F:285:LEU:HD21	2.24	0.67
1:D:193:ARG:HD3	1:D:195:MSE:SE	2.45	0.66
1:D:26:GLU:H	1:D:26:GLU:CD	1.98	0.66
1:C:182:GLN:NE2	1:C:183:ALA:H	1.94	0.66
1:D:303:GLN:HG2	1:D:304:VAL:H	1.61	0.66
1:D:145:MSE:CE	1:D:158:THR:HG23	2.25	0.66
1:E:232:MSE:HE2	1:E:236:VAL:CG2	2.26	0.66
1:F:45:SER:OG	1:F:46:HIS:HD2	1.79	0.66
1:G:303:GLN:HG2	1:G:304:VAL:H	1.61	0.65
1:A:228:TYR:HA	1:A:231:MSE:HE2	1.79	0.65
1:D:227:GLY:O	1:D:231:MSE:HG2	1.96	0.65
1:A:177:MSE:HE3	1:B:230:LEU:HG	1.78	0.65
1:C:306:TYR:CZ	1:C:309:GLN:HG3	2.32	0.65
1:C:2:SER:HB3	1:C:324:GLU:OE2	1.96	0.65
1:A:41:ARG:NE	1:A:311:GLN:HE21	1.95	0.64
1:E:232:MSE:CE	1:E:236:VAL:HG21	2.27	0.64
1:B:321:GLU:HB3	1:H:4:LYS:HZ2	1.62	0.64
1:E:8:GLU:O	1:E:12:GLN:HG2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:273:ASN:ND2	1:E:278:SER:HB3	2.12	0.64
1:E:41:ARG:HH21	1:E:127:GLN:HE22	1.46	0.64
1:D:168:GLU:O	1:D:171:GLU:HB2	1.98	0.64
1:G:125:PHE:HA	1:G:128:GLN:HE21	1.63	0.64
1:G:165:ALA:CB	1:G:285:LEU:HD21	2.28	0.63
1:G:292:LEU:HA	1:G:295:ILE:HD12	1.80	0.63
1:D:73:GLU:HG2	2:D:382:HOH:O	1.98	0.63
1:G:295:ILE:HD13	1:H:148:PRO:HG3	1.81	0.63
1:C:198:PRO:HD2	1:C:201:TRP:CE2	2.34	0.63
1:A:175:PHE:HZ	1:A:177:MSE:HE2	1.64	0.62
1:G:159:ASN:HB3	1:G:234:ILE:HG21	1.80	0.62
1:F:147:VAL:HG12	1:F:153:GLU:O	1.99	0.62
1:B:182:GLN:NE2	1:B:186:LYS:HG3	2.15	0.62
1:G:193:ARG:HD2	1:G:195:MSE:HG2	1.82	0.62
1:A:154:ILE:HD11	1:A:248:ARG:NH2	2.15	0.61
1:C:165:ALA:HB3	1:C:285:LEU:HD21	1.82	0.61
1:D:303:GLN:HG2	1:D:304:VAL:N	2.15	0.61
1:G:303:GLN:HG2	1:G:304:VAL:N	2.15	0.61
1:G:203:VAL:HG11	1:G:207:GLY:HA2	1.83	0.61
1:B:205:LYS:HE2	1:B:205:LYS:H	1.66	0.61
1:E:303:GLN:CG	1:E:304:VAL:H	2.12	0.61
1:D:275:PHE:O	1:D:276:SER:HB3	2.01	0.60
1:D:41:ARG:HD3	1:D:311:GLN:OE1	2.01	0.60
1:F:83:ALA:HB3	1:F:115:ARG:O	2.01	0.60
1:G:145:MSE:CG	2:G:416:HOH:O	2.49	0.60
1:F:194:ASN:HB3	1:G:205:LYS:NZ	2.16	0.60
1:E:193:ARG:HG3	1:E:193:ARG:NH1	2.14	0.60
1:A:303:GLN:HG2	1:A:304:VAL:H	1.66	0.59
1:E:303:GLN:HG2	1:E:304:VAL:N	2.11	0.59
1:E:71:LEU:HD21	1:E:98:HIS:CE1	2.37	0.59
1:A:52:GLU:HG2	1:A:343:TYR:HE1	1.68	0.59
1:F:302:ASN:ND2	1:F:302:ASN:H	2.00	0.59
1:E:143:ASP:CG	1:E:252:SER:HA	2.23	0.59
1:E:193:ARG:O	1:E:195:MSE:N	2.36	0.59
1:E:145:MSE:HE2	1:E:184:TRP:CZ3	2.37	0.59
1:C:202:ALA:HB1	1:C:218:ALA:O	2.02	0.58
1:C:235:ASP:OD1	1:C:246:PHE:HB2	2.03	0.58
1:E:211:THR:O	1:E:211:THR:HG22	2.02	0.58
1:A:277:SER:HB3	1:A:280:LEU:HB2	1.85	0.58
1:E:310:ASP:O	1:E:314:LYS:HG3	2.03	0.58
1:G:324:GLU:HG3	1:G:324:GLU:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:43:ILE:HD11	1:E:311:GLN:NE2	2.19	0.58
1:A:189:ASP:O	1:A:193:ARG:HG2	2.04	0.58
1:F:144:PRO:O	1:F:145:MSE:HG2	2.04	0.58
1:F:159:ASN:H	1:F:159:ASN:ND2	2.02	0.58
1:G:165:ALA:HB1	1:G:285:LEU:HD21	1.86	0.58
1:C:182:GLN:NE2	1:C:186:LYS:HG3	2.19	0.58
1:C:22:GLY:O	1:C:65:ARG:HD2	2.04	0.58
1:E:196:SER:HB2	1:E:211:THR:CG2	2.33	0.57
1:D:12:GLN:NE2	1:H:290:ARG:HE	2.02	0.57
1:E:173:LEU:HD23	1:F:232:MSE:HE3	1.86	0.57
1:B:189:ASP:HB3	1:B:193:ARG:NH1	2.20	0.57
1:E:41:ARG:HH11	1:E:311:GLN:HB3	1.69	0.57
1:D:138:SER:OG	1:D:267:HIS:HD2	1.88	0.57
1:B:303:GLN:HG2	1:B:304:VAL:H	1.70	0.56
1:A:287:GLN:NE2	1:A:291:GLU:OE1	2.33	0.56
1:E:71:LEU:HD21	1:E:98:HIS:ND1	2.20	0.56
1:B:254:TYR:HE1	2:B:448:HOH:O	1.88	0.56
1:C:15:GLU:OE1	1:C:25:ARG:NH1	2.38	0.56
1:C:64:ASN:ND2	1:C:67:PRO:HA	2.21	0.56
1:C:93:LYS:NZ	1:C:124:TYR:OH	2.39	0.56
1:E:228:TYR:HA	1:E:231:MSE:CE	2.36	0.56
1:E:281:PHE:CE2	1:E:285:LEU:HD23	2.41	0.56
1:B:252:SER:HB2	2:B:403:HOH:O	2.06	0.56
1:D:244:LEU:HB3	1:D:245:PRO:HD2	1.87	0.56
1:G:92:ALA:HB2	1:G:116:MSE:HE1	1.88	0.56
1:G:57:ARG:HD3	1:G:62:GLY:O	2.06	0.55
1:H:204:ASP:OD2	1:H:208:VAL:HB	2.07	0.55
1:H:70:ARG:NH1	2:H:443:HOH:O	2.35	0.55
1:A:293:ASN:ND2	1:A:303:GLN:OE1	2.39	0.55
1:B:293:ASN:ND2	1:B:303:GLN:OE1	2.40	0.55
1:C:205:LYS:HD3	1:C:217:HIS:CB	2.32	0.55
1:H:93:LYS:HA	1:H:128:GLN:HE22	1.72	0.55
1:B:167:GLY:O	1:B:282:ARG:NH1	2.40	0.55
1:H:164:ALA:HA	1:H:173:LEU:O	2.06	0.55
1:A:303:GLN:HG2	1:A:304:VAL:N	2.21	0.55
1:G:16:ASN:OD1	1:G:25:ARG:NH2	2.40	0.55
1:F:149:PHE:CD2	1:F:225:PRO:HG3	2.41	0.55
1:E:232:MSE:HE2	1:E:236:VAL:HG21	1.89	0.55
1:E:148:PRO:CG	1:F:295:ILE:HD13	2.35	0.55
1:A:64:ASN:HD21	1:A:67:PRO:HA	1.71	0.54
1:E:226:LYS:HD3	1:F:177:MSE:HE3	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LYS:HZ1	1:A:321:GLU:HB3	1.71	0.54
1:B:193:ARG:C	1:B:195:MSE:N	2.60	0.54
1:E:7:ARG:HG3	1:E:36:VAL:CG1	2.37	0.54
1:A:275:PHE:O	1:A:276:SER:HB3	2.08	0.54
1:E:205:LYS:CE	1:E:205:LYS:H	2.20	0.54
1:B:125:PHE:HA	1:B:128:GLN:HE21	1.73	0.54
1:E:177:MSE:HG3	1:E:177:MSE:O	2.07	0.54
1:E:286:SER:HA	1:E:289:MSE:HE3	1.89	0.54
1:B:344:GLU:OE1	1:B:344:GLU:HA	2.07	0.54
1:A:265:GLN:NE2	1:A:267:HIS:HE1	2.07	0.53
1:B:167:GLY:O	1:B:282:ARG:CZ	2.55	0.53
1:E:180:THR:HG23	1:E:182:GLN:H	1.73	0.53
1:A:168:GLU:O	1:A:171:GLU:HB2	2.09	0.53
1:B:173:LEU:HB2	1:B:289:MSE:HE2	1.90	0.53
1:E:330:TYR:CE2	1:E:334:ILE:HD13	2.43	0.53
1:F:125:PHE:HA	1:F:128:GLN:HE21	1.74	0.53
1:A:125:PHE:HD2	1:A:128:GLN:NE2	2.07	0.53
1:A:232:MSE:HE2	1:A:236:VAL:HG21	1.91	0.53
1:E:182:GLN:CG	1:E:186:LYS:HG2	2.39	0.53
1:A:187:VAL:O	1:A:191:ARG:HB2	2.09	0.53
1:E:123:SER:HB3	1:E:176:ASP:HB2	1.90	0.53
1:E:254:TYR:HB3	1:E:344:GLU:O	2.07	0.53
1:B:303:GLN:HG2	1:B:304:VAL:N	2.24	0.53
1:G:145:MSE:HG3	2:G:416:HOH:O	2.07	0.52
1:B:254:TYR:CE2	1:B:343:TYR:HD2	2.26	0.52
1:B:69:PHE:HB3	1:B:94:MSE:HE1	1.91	0.52
1:G:70:ARG:NH1	2:G:386:HOH:O	2.41	0.52
1:B:321:GLU:HB3	1:H:4:LYS:NZ	2.24	0.52
1:F:37:TYR:OH	1:F:123:SER:HB2	2.09	0.52
1:F:49:VAL:HG23	1:F:329:ILE:HD11	1.91	0.52
1:G:144:PRO:C	1:G:145:MSE:HG2	2.29	0.52
1:A:203:VAL:HA	1:A:209:PRO:HA	1.91	0.52
1:A:20:GLN:NE2	1:A:336:ASP:O	2.37	0.52
1:A:60:LYS:HB3	1:A:258:HIS:CE1	2.45	0.52
1:F:146:VAL:HG11	1:F:231:MSE:HE1	1.92	0.52
1:D:288:THR:HG22	1:D:292:LEU:HD12	1.91	0.52
1:E:2:SER:HA	1:E:327:ASP:OD2	2.08	0.52
1:H:16:ASN:OD1	1:H:25:ARG:NH2	2.43	0.52
1:B:8:GLU:HG2	1:F:290:ARG:CZ	2.40	0.52
1:C:53:TYR:CE2	1:C:253:MSE:HE2	2.45	0.52
1:D:145:MSE:CE	1:D:158:THR:CG2	2.87	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:164:ALA:HA	1:D:173:LEU:O	2.10	0.52
1:F:194:ASN:HB3	1:G:205:LYS:HZ1	1.75	0.52
1:A:205:LYS:HE3	1:A:215:ALA:O	2.11	0.51
1:F:182:GLN:HE21	1:F:183:ALA:H	1.57	0.51
1:F:314:LYS:HE3	2:F:378:HOH:O	2.11	0.51
1:G:7:ARG:HD3	2:G:420:HOH:O	2.10	0.51
1:H:125:PHE:O	1:H:128:GLN:HB2	2.10	0.51
1:A:203:VAL:HG22	1:A:208:VAL:C	2.31	0.51
1:C:233:MSE:HG3	1:D:163:PHE:CD1	2.45	0.51
1:F:202:ALA:HB1	1:F:216:VAL:HG13	1.92	0.51
1:G:131:ARG:NH1	1:G:131:ARG:HG3	2.26	0.51
1:F:193:ARG:NH2	1:H:299:PRO:HG3	2.25	0.51
1:C:203:VAL:HG22	1:C:208:VAL:N	2.25	0.51
1:D:232:MSE:HE2	1:D:236:VAL:HG23	1.86	0.51
1:G:227:GLY:O	1:G:231:MSE:HG3	2.10	0.51
1:D:244:LEU:HB3	1:D:245:PRO:CD	2.40	0.51
1:A:71:LEU:HD21	1:A:98:HIS:ND1	2.26	0.51
1:B:95:GLY:HA3	1:B:113:ILE:CD1	2.40	0.51
1:B:193:ARG:HB2	1:B:195:MSE:HB2	1.92	0.51
1:C:295:ILE:HD12	1:D:148:PRO:HG3	1.93	0.51
1:A:136:GLY:O	1:A:163:PHE:HA	2.11	0.50
1:A:32:ALA:O	1:A:36:VAL:HG23	2.11	0.50
1:C:196:SER:HB2	1:C:211:THR:HG23	1.94	0.50
1:E:2:SER:N	1:E:327:ASP:OD2	2.44	0.50
1:G:173:LEU:CG	1:H:232:MSE:HE3	2.42	0.50
1:C:256:ASP:HA	1:C:344:GLU:OE2	2.12	0.50
1:D:16:ASN:OD1	1:D:25:ARG:NH2	2.42	0.50
1:D:165:ALA:HB3	1:D:285:LEU:HD21	1.94	0.50
1:G:165:ALA:HB3	1:G:285:LEU:HD21	1.93	0.50
1:C:77:CYS:HG	1:D:77:CYS:HG	1.59	0.50
1:E:5:ILE:HD11	1:E:10:LEU:HB2	1.93	0.50
1:G:203:VAL:HG22	1:G:208:VAL:C	2.31	0.50
1:B:144:PRO:O	1:B:145:MSE:HG2	2.12	0.49
1:C:146:VAL:HG11	1:C:231:MSE:HE1	1.93	0.49
1:H:158:THR:O	1:H:159:ASN:C	2.50	0.49
1:D:227:GLY:O	1:D:231:MSE:CG	2.58	0.49
1:A:4:LYS:HZ3	1:A:321:GLU:HB3	1.76	0.49
1:F:56:GLU:HG3	1:F:339:TYR:CE1	2.46	0.49
1:E:275:PHE:O	1:E:276:SER:HB3	2.12	0.49
1:H:8:GLU:CD	1:H:8:GLU:H	2.15	0.49
1:A:248:ARG:HG2	1:A:248:ARG:HH11	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:182:GLN:CD	1:C:186:LYS:HG3	2.33	0.49
1:E:306:TYR:CE1	1:E:309:GLN:HB2	2.47	0.49
1:H:57:ARG:NH1	1:H:259:ALA:O	2.45	0.49
1:H:279:GLU:CD	1:H:279:GLU:H	2.14	0.49
1:B:143:ASP:OD2	1:B:143:ASP:N	2.46	0.49
1:B:282:ARG:HG2	1:B:282:ARG:HH11	1.76	0.49
1:B:71:LEU:HD21	1:B:98:HIS:ND1	2.28	0.49
1:D:62:GLY:HA3	1:D:257:LEU:O	2.12	0.49
1:A:6:SER:OG	1:A:8:GLU:HG2	2.12	0.49
1:C:32:ALA:O	1:C:36:VAL:HG23	2.12	0.49
1:E:143:ASP:OD1	1:E:252:SER:HA	2.13	0.49
1:F:181:VAL:HG22	1:F:222:ALA:HA	1.94	0.49
1:H:5:ILE:HD11	1:H:9:THR:HG22	1.95	0.49
1:A:99:ALA:HB2	1:A:111:VAL:HG21	1.95	0.48
1:B:193:ARG:C	1:B:195:MSE:H	2.16	0.48
1:E:26:GLU:HG3	1:E:27:HIS:CD2	2.48	0.48
1:F:257:LEU:N	1:F:257:LEU:HD22	2.29	0.48
1:G:191:ARG:HG2	1:G:214:PHE:CE2	2.48	0.48
1:A:203:VAL:HG22	1:A:207:GLY:C	2.33	0.48
1:B:173:LEU:HD23	1:B:289:MSE:HG2	1.95	0.48
1:B:166:PRO:HB2	1:B:282:ARG:NH1	2.27	0.48
1:B:282:ARG:NH1	1:B:282:ARG:HG2	2.27	0.48
1:G:37:TYR:CZ	1:G:41:ARG:HD2	2.47	0.48
1:H:277:SER:HG	1:H:279:GLU:HG2	1.77	0.48
1:E:188:LEU:HD23	1:E:191:ARG:HD2	1.95	0.48
1:C:23:LEU:HG	1:C:58:ILE:HD13	1.96	0.48
1:C:65:ARG:HB2	1:C:65:ARG:NH1	2.28	0.48
1:E:232:MSE:HE3	1:F:173:LEU:HD23	1.95	0.48
1:G:3:SER:O	1:G:324:GLU:HA	2.13	0.48
1:C:257:LEU:HD23	1:C:344:GLU:HG3	1.96	0.48
1:C:295:ILE:HG23	1:D:153:GLU:HB2	1.95	0.48
1:D:138:SER:OG	1:D:267:HIS:CD2	2.67	0.48
1:E:308:GLY:O	1:E:312:ASP:OD1	2.31	0.48
1:E:33:GLU:HG2	2:E:404:HOH:O	2.14	0.48
1:G:286:SER:HA	1:G:289:MSE:HE3	1.96	0.48
1:G:191:ARG:HD2	1:G:213:PRO:C	2.34	0.48
1:G:41:ARG:NH2	1:G:312:ASP:OD2	2.47	0.48
1:F:297:PRO:O	1:H:195:MSE:HE3	2.14	0.48
1:D:139:MSE:O	1:D:265:GLN:HG3	2.13	0.48
1:F:303:GLN:HG2	1:F:304:VAL:N	2.29	0.48
1:F:41:ARG:NH2	1:F:311:GLN:HB2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:SER:HB2	1:E:255:ASP:OD2	2.13	0.47
1:G:191:ARG:HD3	1:G:213:PRO:HB2	1.96	0.47
1:C:41:ARG:NH1	1:C:311:GLN:HE21	2.12	0.47
1:F:147:VAL:HG12	1:F:153:GLU:C	2.35	0.47
1:E:110:VAL:HA	1:E:267:HIS:O	2.13	0.47
1:E:7:ARG:NH1	2:E:389:HOH:O	2.46	0.47
1:G:232:MSE:HE1	1:G:236:VAL:HG21	1.91	0.47
1:G:31:VAL:O	1:G:35:LEU:HG	2.15	0.47
1:B:95:GLY:HA3	1:B:113:ILE:HD11	1.97	0.47
1:B:202:ALA:HB1	1:B:216:VAL:HG13	1.97	0.47
1:C:325:ILE:HD13	1:C:330:TYR:HB2	1.97	0.47
1:B:164:ALA:HA	1:B:173:LEU:O	2.15	0.47
1:G:193:ARG:HG2	1:G:193:ARG:NH1	2.30	0.47
1:A:177:MSE:CE	1:B:226:LYS:O	2.62	0.47
1:A:23:LEU:HG	1:A:58:ILE:CD1	2.37	0.47
1:C:55:ALA:O	1:C:59:SER:HB3	2.15	0.47
1:F:325:ILE:HD11	1:F:329:ILE:HG22	1.95	0.47
1:A:196:SER:HB2	1:A:211:THR:HG23	1.96	0.47
1:F:159:ASN:HA	1:F:160:PRO:HD3	1.77	0.47
1:E:303:GLN:CG	1:E:304:VAL:N	2.75	0.47
1:H:189:ASP:O	1:H:193:ARG:HG3	2.15	0.47
1:B:148:PRO:HB3	1:B:228:TYR:CE1	2.50	0.47
1:C:125:PHE:HA	1:C:128:GLN:HE21	1.80	0.47
1:E:193:ARG:C	1:E:195:MSE:H	2.18	0.47
1:G:85:ASN:HA	1:G:115:ARG:O	2.15	0.47
1:H:116:MSE:HE1	1:H:265:GLN:OE1	2.15	0.47
1:D:7:ARG:HG2	1:D:323:ILE:CD1	2.44	0.47
1:E:205:LYS:H	1:E:205:LYS:HE2	1.80	0.47
1:F:302:ASN:N	1:F:302:ASN:ND2	2.63	0.47
1:G:67:PRO:CB	1:G:86:ALA:HB2	2.45	0.47
1:H:224:GLY:HA3	1:H:225:PRO:HD3	1.79	0.47
1:B:292:LEU:HA	1:B:295:ILE:HD12	1.96	0.46
1:F:297:PRO:HG2	1:H:195:MSE:SE	2.65	0.46
1:H:41:ARG:NH1	1:H:311:GLN:OE1	2.48	0.46
1:C:305:TYR:HA	1:C:309:GLN:OE1	2.14	0.46
1:A:175:PHE:CE2	1:A:177:MSE:HE3	2.50	0.46
1:E:68:GLU:HG3	1:E:84:ASP:OD1	2.16	0.46
1:F:164:ALA:HA	1:F:173:LEU:O	2.14	0.46
1:H:280:LEU:HD23	1:H:280:LEU:HA	1.66	0.46
1:F:203:VAL:CG1	1:F:207:GLY:HA2	2.46	0.46
1:B:41:ARG:O	1:B:311:GLN:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:MSE:HG3	1:C:177:MSE:O	2.15	0.46
1:C:325:ILE:HG13	2:C:414:HOH:O	2.15	0.46
1:D:326:VAL:HG22	1:D:329:ILE:HG13	1.98	0.46
1:G:67:PRO:HB3	1:G:86:ALA:HB2	1.97	0.46
1:A:232:MSE:CE	1:A:236:VAL:HG21	2.46	0.46
1:B:179:THR:CB	1:B:231:MSE:HE2	2.46	0.46
1:B:200:THR:O	1:B:220:LEU:HD12	2.16	0.46
1:F:155:TYR:CE1	1:F:248:ARG:HG2	2.51	0.46
1:G:193:ARG:HH11	1:G:193:ARG:CG	2.29	0.46
1:G:4:LYS:HD2	1:G:321:GLU:O	2.14	0.46
1:A:325:ILE:HD11	1:A:329:ILE:HG22	1.97	0.46
1:C:7:ARG:NH1	1:C:40:ALA:HB2	2.31	0.46
1:C:143:ASP:OD2	1:C:261:ARG:NH2	2.47	0.46
1:H:19:CYS:SG	1:H:25:ARG:HA	2.56	0.46
1:H:50:ARG:HH11	1:H:253:MSE:HE1	1.81	0.46
1:B:124:TYR:C	1:B:124:TYR:CD2	2.89	0.46
1:F:177:MSE:HG3	1:F:177:MSE:O	2.15	0.46
1:B:203:VAL:HG22	1:B:207:GLY:C	2.36	0.45
1:C:43:ILE:HD11	1:C:311:GLN:NE2	2.31	0.45
1:E:163:PHE:HE2	1:F:232:MSE:HE1	1.81	0.45
1:H:290:ARG:HD3	2:H:377:HOH:O	2.15	0.45
1:E:116:MSE:O	1:E:263:LEU:HB2	2.16	0.45
1:H:165:ALA:HB3	1:H:285:LEU:HD21	1.97	0.45
1:A:158:THR:O	1:A:159:ASN:C	2.54	0.45
1:C:65:ARG:HH11	1:C:65:ARG:CB	2.28	0.45
1:D:168:GLU:O	1:D:171:GLU:CB	2.65	0.45
1:D:71:LEU:HD21	1:D:98:HIS:ND1	2.30	0.45
1:F:13:LEU:HB3	1:F:333:LEU:HD13	1.99	0.45
1:G:131:ARG:CG	1:G:131:ARG:HH11	2.29	0.45
1:C:107:GLY:HA3	1:C:274:PHE:CD2	2.52	0.45
1:F:108:VAL:CG1	1:F:109:ALA:N	2.79	0.45
1:C:280:LEU:HA	1:C:280:LEU:HD23	1.74	0.45
1:C:163:PHE:HE2	1:D:232:MSE:HE1	1.82	0.45
1:E:153:GLU:HB3	1:E:248:ARG:NH2	2.31	0.45
1:A:164:ALA:HA	1:A:173:LEU:O	2.17	0.45
1:B:244:LEU:HB3	1:B:245:PRO:HD2	1.99	0.45
1:E:254:TYR:CD2	1:E:343:TYR:HB3	2.52	0.45
1:G:285:LEU:HA	1:G:285:LEU:HD12	1.64	0.45
1:G:23:LEU:HG	1:G:58:ILE:HD13	1.99	0.45
1:A:265:GLN:HE21	1:A:267:HIS:HE1	1.63	0.45
1:B:190:ALA:O	1:B:193:ARG:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:240:VAL:HG12	1:D:281:PHE:CD1	2.52	0.45
1:E:273:ASN:ND2	1:E:278:SER:CB	2.80	0.45
1:F:203:VAL:HG22	1:F:208:VAL:C	2.36	0.45
1:H:205:LYS:HB3	1:H:205:LYS:HZ2	1.82	0.45
1:H:62:GLY:HA3	1:H:257:LEU:O	2.17	0.45
1:B:173:LEU:HD23	1:B:289:MSE:CG	2.46	0.44
1:C:123:SER:HA	1:C:126:VAL:HG22	1.99	0.44
1:C:1:SER:HA	1:C:327:ASP:OD2	2.17	0.44
1:F:158:THR:HG22	1:F:180:THR:HG21	1.98	0.44
1:F:244:LEU:O	1:F:245:PRO:C	2.51	0.44
1:G:125:PHE:HA	1:G:128:GLN:NE2	2.31	0.44
1:H:235:ASP:OD1	1:H:246:PHE:HB2	2.16	0.44
1:A:193:ARG:O	1:A:195:MSE:HG3	2.17	0.44
1:D:280:LEU:HD23	1:D:283:GLN:NE2	2.32	0.44
1:F:235:ASP:OD1	1:F:246:PHE:HB2	2.17	0.44
1:G:191:ARG:HD2	1:G:214:PHE:HA	2.00	0.44
1:G:50:ARG:HE	1:G:253:MSE:HE3	1.83	0.44
1:A:228:TYR:HA	1:A:231:MSE:CE	2.45	0.44
1:C:121:ALA:HB1	2:C:425:HOH:O	2.17	0.44
1:E:110:VAL:HG22	1:E:268:ILE:HG12	1.99	0.44
1:H:50:ARG:NH1	1:H:253:MSE:HE1	2.32	0.44
1:D:24:LYS:HB3	1:D:26:GLU:OE2	2.17	0.44
1:E:181:VAL:HG22	1:E:222:ALA:HA	1.99	0.44
1:E:41:ARG:NH1	1:E:311:GLN:CB	2.80	0.44
1:F:261:ARG:O	1:F:262:ASN:HB2	2.17	0.44
1:H:145:MSE:HE1	1:H:184:TRP:CD1	2.52	0.44
1:B:62:GLY:HA3	1:B:257:LEU:O	2.17	0.44
1:C:107:GLY:O	1:C:108:VAL:HG23	2.17	0.44
1:D:188:LEU:HD23	1:D:191:ARG:HD2	1.99	0.44
1:E:182:GLN:HG2	1:E:186:LYS:HG2	2.00	0.44
1:A:67:PRO:HB3	1:A:86:ALA:HB2	2.00	0.44
1:B:204:ASP:OD1	1:B:206:ASN:N	2.48	0.44
1:D:23:LEU:HG	1:D:58:ILE:HD13	1.99	0.44
1:D:283:GLN:NE2	2:D:463:HOH:O	2.09	0.44
1:G:203:VAL:HG22	1:G:209:PRO:N	2.32	0.44
1:C:221:PRO:HB3	1:C:231:MSE:HE1	2.00	0.44
1:E:41:ARG:NH1	1:E:311:GLN:HB3	2.33	0.44
1:A:148:PRO:HB3	1:A:228:TYR:CE1	2.53	0.44
1:B:179:THR:HB	1:B:231:MSE:HE2	1.99	0.44
1:B:182:GLN:HE21	1:B:183:ALA:H	1.66	0.44
1:B:65:ARG:HG3	1:B:66:GLU:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:232:MSE:HE2	1:G:236:VAL:HG23	1.92	0.44
1:E:305:TYR:HB3	1:E:309:GLN:HB3	2.00	0.44
1:F:194:ASN:O	1:F:194:ASN:CG	2.56	0.44
1:A:154:ILE:HD11	1:A:248:ARG:CZ	2.48	0.43
1:A:303:GLN:HB3	1:A:303:GLN:HE21	1.44	0.43
1:B:213:PRO:HA	1:B:216:VAL:HG23	2.00	0.43
1:C:203:VAL:HG22	1:C:208:VAL:C	2.38	0.43
1:D:246:PHE:H	1:D:249:GLN:HE21	1.66	0.43
1:E:101:LYS:O	1:E:104:GLN:HB2	2.18	0.43
1:G:338:LEU:HA	1:G:338:LEU:HD23	1.71	0.43
1:E:198:PRO:HD2	1:E:201:TRP:CD2	2.53	0.43
1:E:327:ASP:HB2	2:E:385:HOH:O	2.17	0.43
1:E:34:VAL:HB	1:E:89:GLN:HG2	2.00	0.43
1:F:57:ARG:HG2	1:F:63:THR:OG1	2.18	0.43
1:G:137:ILE:HB	1:G:268:ILE:HB	2.00	0.43
1:G:76:PRO:O	1:G:106:ASN:ND2	2.50	0.43
1:A:122:ILE:HG21	1:A:122:ILE:HD13	1.74	0.43
1:A:175:PHE:CZ	1:A:177:MSE:CE	3.01	0.43
1:B:125:PHE:O	1:B:128:GLN:HB2	2.18	0.43
1:G:85:ASN:N	1:G:115:ARG:O	2.49	0.43
1:H:232:MSE:HE2	1:H:236:VAL:HG21	2.00	0.43
1:B:122:ILE:HG13	1:B:162:ALA:HB2	2.01	0.43
1:C:203:VAL:HG23	1:C:209:PRO:N	2.33	0.43
1:D:14:ILE:HG12	1:D:51:VAL:HG21	2.01	0.43
1:D:191:ARG:HG3	1:D:213:PRO:HB2	2.00	0.43
1:D:224:GLY:HA3	1:D:225:PRO:HD3	1.89	0.43
1:E:193:ARG:C	1:E:195:MSE:N	2.72	0.43
1:B:325:ILE:HD11	1:B:329:ILE:HG22	2.00	0.43
1:A:232:MSE:HE3	1:B:173:LEU:CG	2.23	0.43
1:B:205:LYS:HE2	1:B:205:LYS:N	2.33	0.43
1:E:93:LYS:O	1:E:97:GLU:HG3	2.18	0.43
1:G:193:ARG:O	1:G:194:ASN:HB2	2.19	0.43
1:A:139:MSE:HG3	1:A:234:ILE:HG23	2.00	0.43
1:A:99:ALA:HB2	1:A:111:VAL:CG2	2.49	0.43
1:C:229:GLY:HA3	1:D:175:PHE:CE1	2.54	0.43
1:E:212:ASP:HA	1:E:213:PRO:HD2	1.89	0.43
1:E:232:MSE:HE3	1:F:173:LEU:HD21	1.99	0.43
1:E:182:GLN:NE2	1:E:186:LYS:HD3	2.34	0.43
1:E:2:SER:CA	1:E:327:ASP:OD2	2.66	0.43
1:F:224:GLY:HA3	1:F:225:PRO:HD3	1.90	0.43
1:G:203:VAL:CG1	1:G:207:GLY:HA2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:ASN:HA	1:D:293:ASN:HD22	1.67	0.43
1:A:338:LEU:O	1:A:339:TYR:HB3	2.18	0.43
1:C:173:LEU:HD23	1:D:232:MSE:CE	2.27	0.43
1:D:145:MSE:HE2	2:D:353:HOH:O	2.19	0.43
1:E:148:PRO:HD3	1:E:153:GLU:O	2.18	0.43
1:E:137:ILE:HG12	1:E:163:PHE:HD1	1.83	0.43
1:F:125:PHE:O	1:F:128:GLN:HB2	2.18	0.43
1:F:56:GLU:HG3	1:F:339:TYR:CD1	2.54	0.43
1:A:18:LEU:HA	1:A:18:LEU:HD12	1.80	0.42
1:B:211:THR:CG2	1:B:211:THR:O	2.66	0.42
1:B:166:PRO:HB2	1:B:282:ARG:HH11	1.84	0.42
1:D:45:SER:OG	1:D:46:HIS:HD2	2.02	0.42
1:A:175:PHE:CZ	1:B:229:GLY:HA3	2.54	0.42
1:A:325:ILE:HG13	1:A:326:VAL:N	2.34	0.42
1:B:137:ILE:HB	1:B:268:ILE:HB	2.02	0.42
1:C:203:VAL:CG2	1:C:208:VAL:C	2.87	0.42
1:E:203:VAL:HG13	1:E:204:ASP:O	2.18	0.42
1:E:179:THR:OG1	1:E:231:MSE:HG2	2.19	0.42
1:E:304:VAL:N	2:E:376:HOH:O	2.46	0.42
1:G:305:TYR:HD2	1:G:309:GLN:OE1	2.02	0.42
1:C:92:ALA:HB3	1:C:125:PHE:CZ	2.54	0.42
1:D:331:GLN:HG2	2:D:452:HOH:O	2.18	0.42
1:H:158:THR:HG22	1:H:180:THR:OG1	2.19	0.42
1:E:232:MSE:HE1	1:E:236:VAL:HG21	1.99	0.42
1:G:173:LEU:HD21	1:H:232:MSE:HE3	1.93	0.42
1:B:232:MSE:HE2	1:B:236:VAL:HG23	1.98	0.42
1:D:116:MSE:HE1	1:D:119:SER:OG	2.19	0.42
1:D:182:GLN:HE21	1:D:186:LYS:HG3	1.85	0.42
1:D:228:TYR:HA	1:D:231:MSE:HG3	2.00	0.42
1:F:41:ARG:HD3	1:F:41:ARG:HH11	1.68	0.42
1:H:336:ASP:N	1:H:336:ASP:OD1	2.52	0.42
1:A:302:ASN:O	1:A:303:GLN:HB2	2.20	0.42
1:A:175:PHE:CE1	1:B:229:GLY:HA3	2.55	0.42
1:E:292:LEU:HA	1:E:292:LEU:HD23	1.93	0.42
1:F:14:ILE:HG12	1:F:51:VAL:HG21	2.02	0.42
1:F:78:SER:HA	1:F:110:VAL:O	2.20	0.42
1:H:191:ARG:HG2	1:H:214:PHE:CE1	2.54	0.42
1:B:231:MSE:SE	2:B:397:HOH:O	2.88	0.42
1:B:330:TYR:CE2	1:B:334:ILE:HD13	2.55	0.42
1:C:60:LYS:NZ	2:C:406:HOH:O	2.44	0.42
1:D:10:LEU:HG	1:D:36:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:181:VAL:HB	2:G:385:HOH:O	2.19	0.42
1:F:275:PHE:O	1:F:276:SER:HB3	2.20	0.42
1:G:143:ASP:OD2	1:G:143:ASP:N	2.53	0.42
1:B:193:ARG:O	1:B:194:ASN:C	2.57	0.41
1:C:213:PRO:HA	1:C:216:VAL:HG23	2.02	0.41
1:C:212:ASP:HA	1:C:213:PRO:HD2	1.96	0.41
1:C:338:LEU:HD23	1:C:338:LEU:HA	1.88	0.41
1:H:205:LYS:HB3	1:H:205:LYS:HZ3	1.82	0.41
1:A:253:MSE:HE2	1:A:254:TYR:CE2	2.55	0.41
1:E:275:PHE:HA	1:F:80:ILE:HD11	2.01	0.41
1:A:5:ILE:HD11	1:A:10:LEU:HD13	2.01	0.41
1:B:8:GLU:HG2	1:F:290:ARG:NE	2.34	0.41
1:H:230:LEU:HA	1:H:230:LEU:HD23	1.80	0.41
1:B:296:THR:OG1	1:D:193:ARG:NH2	2.53	0.41
1:B:306:TYR:CZ	1:B:309:GLN:HB2	2.56	0.41
1:E:10:LEU:CD2	1:E:36:VAL:HG22	2.50	0.41
1:F:309:GLN:O	1:F:312:ASP:HB2	2.21	0.41
1:G:5:ILE:CG1	1:G:9:THR:HB	2.49	0.41
1:A:248:ARG:HG2	1:A:248:ARG:NH1	2.35	0.41
1:E:51:VAL:HG11	1:E:333:LEU:HD21	2.02	0.41
1:F:193:ARG:O	1:F:194:ASN:C	2.58	0.41
1:G:77:CYS:SG	1:G:106:ASN:HB3	2.60	0.41
1:H:261:ARG:O	1:H:262:ASN:HB2	2.20	0.41
1:A:101:LYS:HD3	1:A:102:THR:N	2.36	0.41
1:A:7:ARG:HH11	1:A:319:ALA:HB2	1.86	0.41
1:D:181:VAL:HG22	1:D:222:ALA:HA	2.02	0.41
1:D:324:GLU:H	1:D:324:GLU:HG2	1.46	0.41
1:E:198:PRO:HD2	1:E:201:TRP:CE2	2.54	0.41
1:F:186:LYS:HB3	1:F:201:TRP:CZ3	2.55	0.41
1:H:338:LEU:HA	1:H:338:LEU:HD23	1.91	0.41
1:A:291:GLU:O	1:A:295:ILE:HG12	2.20	0.41
1:E:125:PHE:HA	1:E:128:GLN:HE21	1.85	0.41
1:E:203:VAL:HG22	1:E:208:VAL:C	2.41	0.41
1:G:187:VAL:HG11	1:G:216:VAL:HG11	2.03	0.41
1:A:265:GLN:HE21	1:A:267:HIS:CE1	2.39	0.41
1:B:235:ASP:OD1	1:B:246:PHE:HB2	2.21	0.41
1:C:22:GLY:C	1:C:65:ARG:HD2	2.41	0.41
1:C:175:PHE:CE1	1:D:229:GLY:HA3	2.56	0.41
1:F:244:LEU:HD12	1:F:264:GLY:HA3	2.03	0.41
1:G:147:VAL:HG12	1:G:153:GLU:O	2.21	0.41
1:G:83:ALA:HB3	1:G:115:ARG:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:PHE:CZ	1:A:177:MSE:HE2	2.50	0.41
1:B:179:THR:OG1	1:B:231:MSE:HE2	2.20	0.41
1:B:237:LEU:HB3	1:B:266:LEU:HD22	2.03	0.41
1:C:163:PHE:CD1	1:D:233:MSE:HG3	2.56	0.41
1:D:5:ILE:HD13	1:D:5:ILE:HG21	1.85	0.41
1:F:136:GLY:O	1:F:163:PHE:HA	2.20	0.41
1:G:50:ARG:NH2	1:G:118:HIS:CE1	2.89	0.41
1:G:173:LEU:HD22	1:G:289:MSE:HG3	2.03	0.41
1:H:39:ASP:HB3	1:H:323:ILE:HG21	2.03	0.41
1:E:187:VAL:O	1:E:191:ARG:HG3	2.21	0.41
1:E:291:GLU:O	1:E:295:ILE:HD13	2.21	0.41
1:E:171:GLU:O	1:E:172:ILE:HG13	2.21	0.40
1:E:182:GLN:HE21	1:E:186:LYS:HD3	1.85	0.40
1:E:304:VAL:HB	2:E:376:HOH:O	2.20	0.40
1:G:303:GLN:HG2	2:G:384:HOH:O	2.21	0.40
1:A:303:GLN:NE2	1:A:305:TYR:CE1	2.89	0.40
1:A:67:PRO:CB	1:A:86:ALA:HB2	2.52	0.40
1:C:204:ASP:OD1	1:C:206:ASN:N	2.53	0.40
1:D:130:ALA:HA	1:D:134:PHE:O	2.20	0.40
1:F:57:ARG:NH1	1:F:259:ALA:O	2.54	0.40
1:C:176:ASP:OD1	2:C:425:HOH:O	2.22	0.40
1:D:253:MSE:HB3	1:D:254:TYR:CD1	2.57	0.40
1:G:131:ARG:CG	1:G:131:ARG:NH1	2.82	0.40
1:G:159:ASN:HA	1:G:160:PRO:HD2	2.01	0.40
1:G:69:PHE:CG	1:G:94:MSE:HE1	2.55	0.40
1:H:7:ARG:HG3	1:H:36:VAL:HG11	2.03	0.40
1:B:310:ASP:HB3	2:B:446:HOH:O	2.20	0.40
1:E:10:LEU:HD23	1:E:36:VAL:HG22	2.03	0.40
1:F:165:ALA:HB3	1:F:285:LEU:CD2	2.43	0.40
1:E:229:GLY:HA3	1:F:175:PHE:CE1	2.56	0.40
1:F:295:ILE:HG22	1:F:304:VAL:HG21	2.03	0.40
1:H:34:VAL:HG12	2:H:356:HOH:O	2.22	0.40
1:D:158:THR:O	1:D:159:ASN:C	2.60	0.40
1:E:302:ASN:O	1:E:303:GLN:HB2	2.21	0.40
1:G:158:THR:HG22	1:G:180:THR:CG2	2.47	0.40
1:H:321:GLU:HA	1:H:321:GLU:OE2	2.22	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	341/351 (97%)	317 (93%)	21 (6%)	3 (1%)	17	14
1	B	341/351 (97%)	323 (95%)	14 (4%)	4 (1%)	13	9
1	C	342/351 (97%)	332 (97%)	9 (3%)	1 (0%)	41	46
1	D	340/351 (97%)	329 (97%)	9 (3%)	2 (1%)	25	25
1	E	341/351 (97%)	319 (94%)	20 (6%)	2 (1%)	25	25
1	F	337/351 (96%)	321 (95%)	12 (4%)	4 (1%)	13	9
1	G	339/351 (97%)	326 (96%)	12 (4%)	1 (0%)	41	46
1	H	337/351 (96%)	325 (96%)	10 (3%)	2 (1%)	25	25
All	All	2718/2808 (97%)	2592 (95%)	107 (4%)	19 (1%)	22	21

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	195	MSE
1	E	194	ASN
1	B	192	SER
1	B	194	ASN
1	G	194	ASN
1	F	199	ASP
1	A	159	ASN
1	A	194	ASN
1	B	159	ASN
1	D	159	ASN
1	D	276	SER
1	C	159	ASN
1	E	159	ASN
1	F	159	ASN
1	F	194	ASN
1	H	159	ASN
1	A	239	GLY

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Mol	Chain	Res	Type
1	F	239	GLY
1	H	239	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	272/267 (102%)	248 (91%)	24 (9%)	10	8
1	B	272/267 (102%)	256 (94%)	16 (6%)	19	19
1	C	273/267 (102%)	259 (95%)	14 (5%)	24	25
1	D	271/267 (102%)	249 (92%)	22 (8%)	11	10
1	E	272/267 (102%)	252 (93%)	20 (7%)	13	12
1	F	268/267 (100%)	244 (91%)	24 (9%)	9	7
1	G	270/267 (101%)	253 (94%)	17 (6%)	18	17
1	H	268/267 (100%)	256 (96%)	12 (4%)	27	31
All	All	2166/2136 (101%)	2017 (93%)	149 (7%)	15	14

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	18	LEU
1	A	19	CYS
1	A	25	ARG
1	A	59	SER
1	A	65	ARG
1	A	97	GLU
1	A	104	GLN
1	A	153	GLU
1	A	192	SER
1	A	193	ARG
1	A	194	ASN
1	A	203	VAL

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Mol	Chain	Res	Type
1	A	205	LYS
1	A	248	ARG
1	A	279	GLU
1	A	285	LEU
1	A	293	ASN
1	A	302	ASN
1	A	303	GLN
1	A	310	ASP
1	A	317	LYS
1	A	325	ILE
1	A	344	GLU
1	B	18	LEU
1	B	19	CYS
1	B	33	GLU
1	B	68	GLU
1	B	101	LYS
1	B	108	VAL
1	B	138	SER
1	B	143	ASP
1	B	173	LEU
1	B	191	ARG
1	B	203	VAL
1	B	205	LYS
1	B	252	SER
1	B	283	GLN
1	B	331	GLN
1	B	344	GLU
1	C	9	THR
1	C	10	LEU
1	C	18	LEU
1	C	19	CYS
1	C	26	GLU
1	C	59	SER
1	C	97	GLU
1	C	104	GLN
1	C	203	VAL
1	C	257	LEU
1	C	285	LEU
1	C	303	GLN
1	C	324	GLU
1	C	328	ASP
1	D	3	SER

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Mol	Chain	Res	Type
1	D	4	LYS
1	D	18	LEU
1	D	19	CYS
1	D	33	GLU
1	D	50	ARG
1	D	65	ARG
1	D	66	GLU
1	D	68	GLU
1	D	73	GLU
1	D	143	ASP
1	D	192	SER
1	D	194	ASN
1	D	211	THR
1	D	230	LEU
1	D	231	MSE
1	D	232	MSE
1	D	253	MSE
1	D	266	LEU
1	D	279	GLU
1	D	324	GLU
1	D	326	VAL
1	E	3	SER
1	E	18	LEU
1	E	24	LYS
1	E	33	GLU
1	E	65	ARG
1	E	104	GLN
1	E	108	VAL
1	E	180	THR
1	E	186	LYS
1	E	193	ARG
1	E	195	MSE
1	E	203	VAL
1	E	205	LYS
1	E	263	LEU
1	E	285	LEU
1	E	293	ASN
1	E	303	GLN
1	E	310	ASP
1	E	336	ASP
1	E	341	THR
1	F	2	SER

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Mol	Chain	Res	Type
1	F	3	SER
1	F	18	LEU
1	F	19	CYS
1	F	37	TYR
1	F	50	ARG
1	F	52	GLU
1	F	65	ARG
1	F	66	GLU
1	F	68	GLU
1	F	123	SER
1	F	127	GLN
1	F	128	GLN
1	F	143	ASP
1	F	145	MSE
1	F	173	LEU
1	F	179	THR
1	F	203	VAL
1	F	210	THR
1	F	232	MSE
1	F	248	ARG
1	F	302	ASN
1	F	327	ASP
1	F	328	ASP
1	G	3	SER
1	G	18	LEU
1	G	19	CYS
1	G	25	ARG
1	G	65	ARG
1	G	131	ARG
1	G	145	MSE
1	G	173	LEU
1	G	193	ARG
1	G	194	ASN
1	G	195	MSE
1	G	211	THR
1	G	232	MSE
1	G	273	ASN
1	G	279	GLU
1	G	324	GLU
1	G	336	ASP
1	H	25	ARG
1	H	59	SER

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Mol	Chain	Res	Type
1	H	97	GLU
1	H	105	GLN
1	H	141	GLN
1	H	143	ASP
1	H	203	VAL
1	H	206	ASN
1	H	279	GLU
1	H	285	LEU
1	H	317	LYS
1	H	327	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	182	GLN
1	A	206	ASN
1	A	293	ASN
1	A	303	GLN
1	A	311	GLN
1	B	20	GLN
1	B	128	GLN
1	B	182	GLN
1	B	206	ASN
1	B	273	ASN
1	B	283	GLN
1	B	293	ASN
1	C	11	HIS
1	C	12	GLN
1	C	128	GLN
1	C	182	GLN
1	C	206	ASN
1	C	303	GLN
1	C	311	GLN
1	D	11	HIS
1	D	12	GLN
1	D	46	HIS
1	D	182	GLN
1	D	206	ASN
1	D	249	GLN
1	D	265	GLN
1	D	267	HIS

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Mol	Chain	Res	Type
1	D	303	GLN
1	D	331	GLN
1	E	127	GLN
1	E	128	GLN
1	E	182	GLN
1	E	273	ASN
1	E	303	GLN
1	E	311	GLN
1	E	331	GLN
1	F	46	HIS
1	F	128	GLN
1	F	159	ASN
1	F	182	GLN
1	F	249	GLN
1	F	302	ASN
1	F	303	GLN
1	F	311	GLN
1	F	331	GLN
1	G	11	HIS
1	G	46	HIS
1	G	128	GLN
1	G	159	ASN
1	G	194	ASN
1	G	273	ASN
1	G	293	ASN
1	G	303	GLN
1	H	46	HIS
1	H	104	GLN
1	H	128	GLN
1	H	182	GLN
1	H	206	ASN
1	H	273	ASN
1	H	293	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides 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 [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	331/351 (94%)	0.08	10 (3%) 50 53	25, 40, 59, 75	0
1	B	331/351 (94%)	-0.07	7 (2%) 63 66	21, 33, 54, 70	0
1	C	332/351 (94%)	-0.01	11 (3%) 46 48	19, 37, 53, 68	0
1	D	330/351 (94%)	-0.14	4 (1%) 79 81	21, 34, 50, 67	0
1	E	331/351 (94%)	0.06	18 (5%) 25 28	21, 37, 59, 75	0
1	F	327/351 (93%)	-0.08	4 (1%) 79 81	24, 38, 54, 67	0
1	G	329/351 (93%)	-0.00	10 (3%) 50 53	22, 35, 58, 73	0
1	H	327/351 (93%)	-0.09	6 (1%) 68 71	19, 32, 55, 65	0
All	All	2638/2808 (93%)	-0.03	70 (2%) 54 57	19, 36, 56, 75	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	SER	6.2
1	B	341	THR	4.9
1	E	344	GLU	4.5
1	E	343	TYR	4.4
1	G	341	THR	4.2
1	G	342	SER	4.1
1	D	2	SER	4.1
1	G	214	PHE	4.1
1	E	342	SER	3.9
1	G	192	SER	3.7
1	G	340	ASN	3.7
1	E	341	THR	3.4
1	E	300	GLY	3.3
1	B	2	SER	3.3
1	C	2	SER	3.2
1	A	192	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	255	ASP	3.2
1	H	254	TYR	3.1
1	G	2	SER	3.1
1	D	336	ASP	3.1
1	F	254	TYR	3.1
1	A	2	SER	3.1
1	C	343	TYR	3.0
1	C	333	LEU	3.0
1	E	340	ASN	2.9
1	B	254	TYR	2.9
1	E	193	ARG	2.9
1	G	194	ASN	2.9
1	A	66	GLU	2.8
1	G	302	ASN	2.8
1	C	341	THR	2.8
1	E	170	ASP	2.7
1	A	193	ARG	2.7
1	E	194	ASN	2.7
1	A	194	ASN	2.6
1	H	340	ASN	2.6
1	E	320	VAL	2.6
1	C	328	ASP	2.6
1	B	343	TYR	2.6
1	D	192	SER	2.5
1	B	192	SER	2.5
1	E	319	ALA	2.5
1	E	205	LYS	2.5
1	F	340	ASN	2.4
1	H	173	LEU	2.4
1	A	189	ASP	2.4
1	A	302	ASN	2.4
1	E	214	PHE	2.3
1	E	273	ASN	2.3
1	D	254	TYR	2.3
1	C	344	GLU	2.3
1	F	2	SER	2.3
1	G	327	ASP	2.2
1	E	192	SER	2.2
1	B	336	ASP	2.2
1	C	340	ASN	2.2
1	C	336	ASP	2.2
1	F	58	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	2	SER	2.1
1	H	206	ASN	2.1
1	B	146	VAL	2.1
1	A	169	GLY	2.1
1	C	342	SER	2.1
1	E	336	ASP	2.1
1	C	66	GLU	2.1
1	H	18	LEU	2.0
1	A	215	ALA	2.0
1	E	303	GLN	2.0
1	G	203	VAL	2.0
1	H	214	PHE	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 monosaccharides 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.