



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 05:11 pm BST

PDB ID : 5XTW
Title : Crystal structure of the CysR-CTLD2 fragment of human MR at acidic pH
Authors : He, Y.; Hu, Z.
Deposited on : 2017-06-21
Resolution : 3.20 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 : 2.11
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) : 2.11

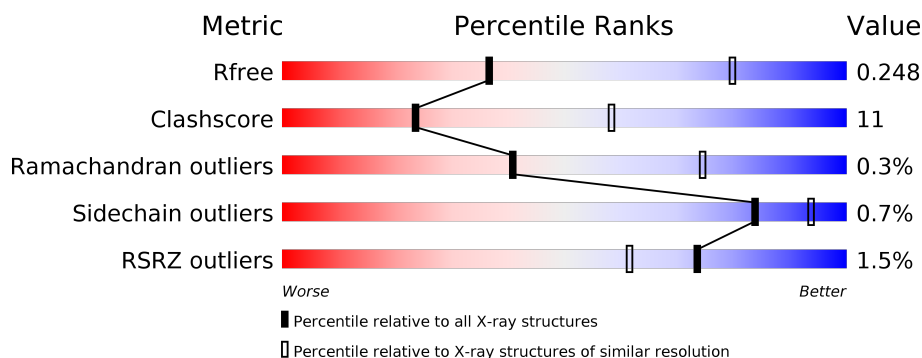
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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 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	475	<div> <div>%</div> <div> <div></div> <div>69%</div> <div>24%</div> <div>7%</div> </div> </div>
1	B	475	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>21%</div> <div>7%</div> </div> </div>
1	C	475	<div> <div>%</div> <div> <div></div> <div>67%</div> <div>25%</div> <div>7%</div> </div> </div>
1	D	475	<div> <div>%</div> <div> <div></div> <div>70%</div> <div>23%</div> <div>7%</div> </div> </div>
1	E	475	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>22%</div> <div>7%</div> </div> </div>
1	F	475	<div> <div>%</div> <div> <div></div> <div>72%</div> <div>21%</div> <div>7%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	475	<div><div><div>%</div><div><div></div><div>74%</div><div>19%</div><div>7%</div></div></div></div>
1	H	475	<div><div><div>2%</div><div><div></div><div>66%</div><div>26%</div><div>7%</div></div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28716 atoms, of which 104 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 Macrophage mannose receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	443	Total	C	N	O	S	0	0	0
			3570	2267	602	676	25			
1	B	443	Total	C	N	O	S	0	0	0
			3570	2267	602	676	25			
1	C	441	Total	C	N	O	S	0	0	0
			3549	2256	595	673	25			
1	D	443	Total	C	N	O	S	0	0	0
			3570	2267	602	676	25			
1	E	444	Total	C	N	O	S	0	0	0
			3577	2271	603	678	25			
1	F	442	Total	C	N	O	S	0	0	0
			3561	2263	599	674	25			
1	G	443	Total	C	N	O	S	0	0	0
			3563	2260	601	677	25			
1	H	441	Total	C	N	O	S	0	0	0
			3550	2257	595	673	25			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	491	HIS	-	expression tag	UNP P22897
A	492	HIS	-	expression tag	UNP P22897
A	493	HIS	-	expression tag	UNP P22897
A	494	HIS	-	expression tag	UNP P22897
A	495	HIS	-	expression tag	UNP P22897
A	496	HIS	-	expression tag	UNP P22897
B	491	HIS	-	expression tag	UNP P22897
B	492	HIS	-	expression tag	UNP P22897
B	493	HIS	-	expression tag	UNP P22897
B	494	HIS	-	expression tag	UNP P22897
B	495	HIS	-	expression tag	UNP P22897
B	496	HIS	-	expression tag	UNP P22897
C	491	HIS	-	expression tag	UNP P22897

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Chain	Residue	Modelled	Actual	Comment	Reference
C	492	HIS	-	expression tag	UNP P22897
C	493	HIS	-	expression tag	UNP P22897
C	494	HIS	-	expression tag	UNP P22897
C	495	HIS	-	expression tag	UNP P22897
C	496	HIS	-	expression tag	UNP P22897
D	491	HIS	-	expression tag	UNP P22897
D	492	HIS	-	expression tag	UNP P22897
D	493	HIS	-	expression tag	UNP P22897
D	494	HIS	-	expression tag	UNP P22897
D	495	HIS	-	expression tag	UNP P22897
D	496	HIS	-	expression tag	UNP P22897
E	491	HIS	-	expression tag	UNP P22897
E	492	HIS	-	expression tag	UNP P22897
E	493	HIS	-	expression tag	UNP P22897
E	494	HIS	-	expression tag	UNP P22897
E	495	HIS	-	expression tag	UNP P22897
E	496	HIS	-	expression tag	UNP P22897
F	491	HIS	-	expression tag	UNP P22897
F	492	HIS	-	expression tag	UNP P22897
F	493	HIS	-	expression tag	UNP P22897
F	494	HIS	-	expression tag	UNP P22897
F	495	HIS	-	expression tag	UNP P22897
F	496	HIS	-	expression tag	UNP P22897
G	491	HIS	-	expression tag	UNP P22897
G	492	HIS	-	expression tag	UNP P22897
G	493	HIS	-	expression tag	UNP P22897
G	494	HIS	-	expression tag	UNP P22897
G	495	HIS	-	expression tag	UNP P22897
G	496	HIS	-	expression tag	UNP P22897
H	491	HIS	-	expression tag	UNP P22897
H	492	HIS	-	expression tag	UNP P22897
H	493	HIS	-	expression tag	UNP P22897
H	494	HIS	-	expression tag	UNP P22897
H	495	HIS	-	expression tag	UNP P22897
H	496	HIS	-	expression tag	UNP P22897

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
2	B	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
2	C	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
2	D	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
2	E	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
2	F	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
2	G	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		
2	H	1	Total	C	H	N	O	S	0	0
			25	6	13	1	4	1		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Ca	0	0
			1	1		
3	E	1	Total	Ca	0	0
			1	1		
3	H	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

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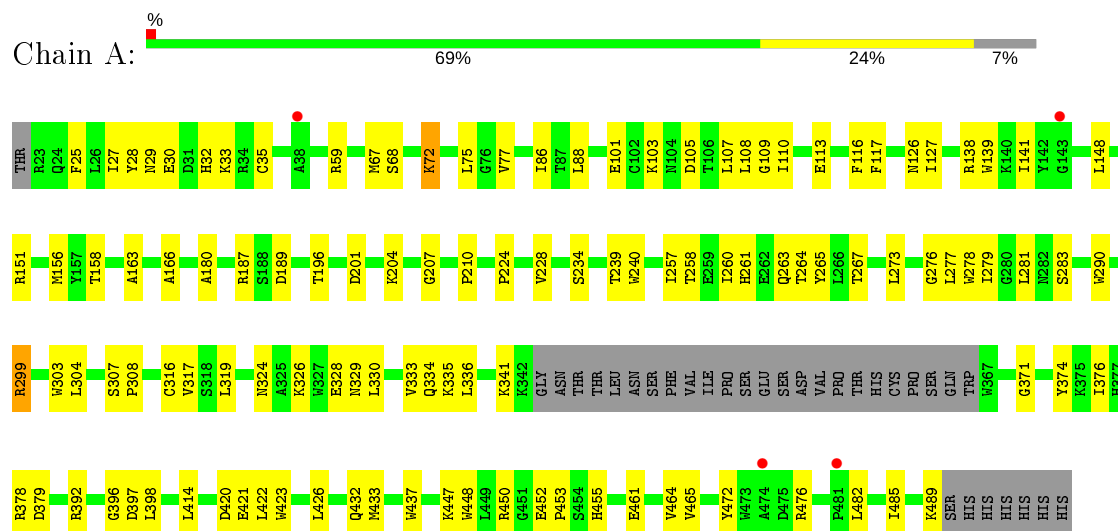
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Ca 1	0	0
3	F	1	Total 1	Ca 1	0	0

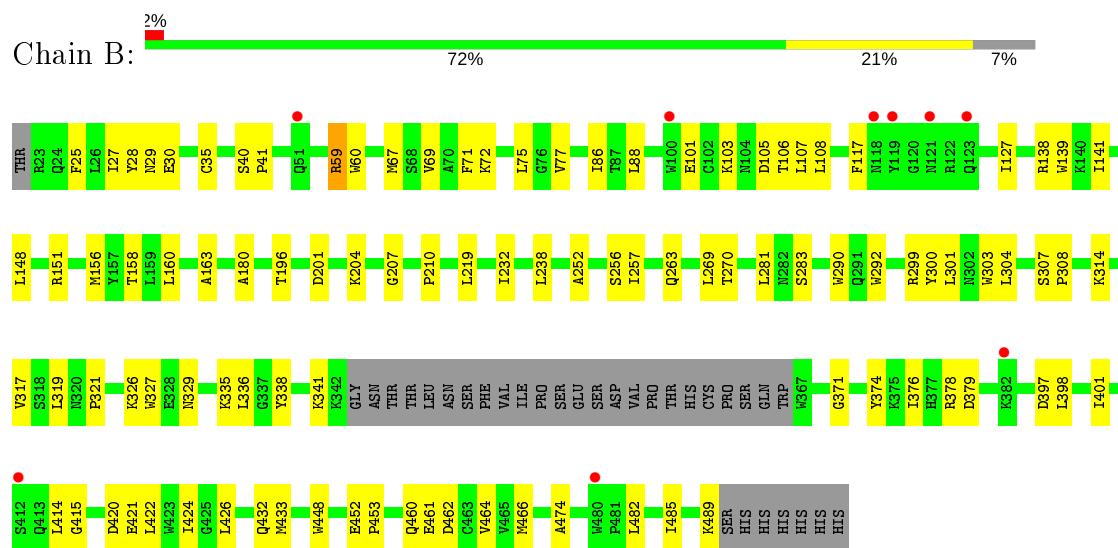
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Macrophage mannose receptor 1



• Molecule 1: Macrophage mannose receptor 1

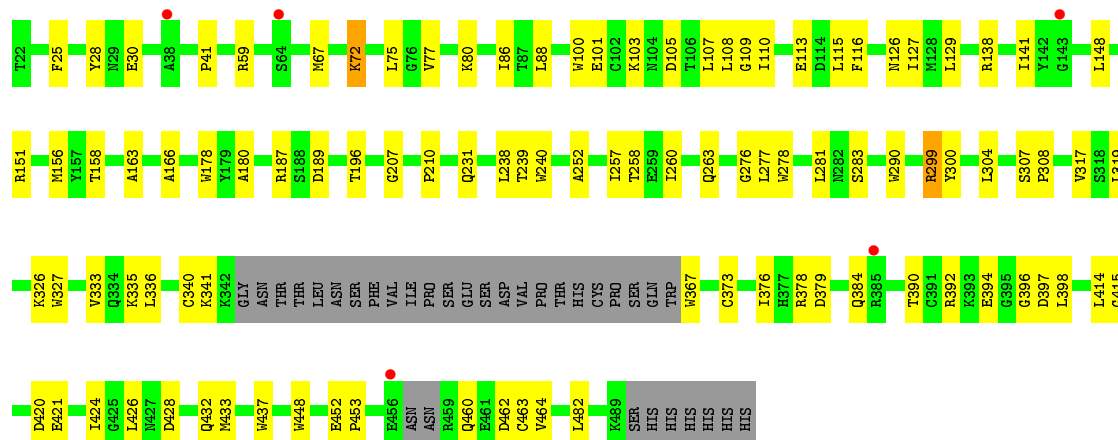


• Molecule 1: Macrophage mannose receptor 1

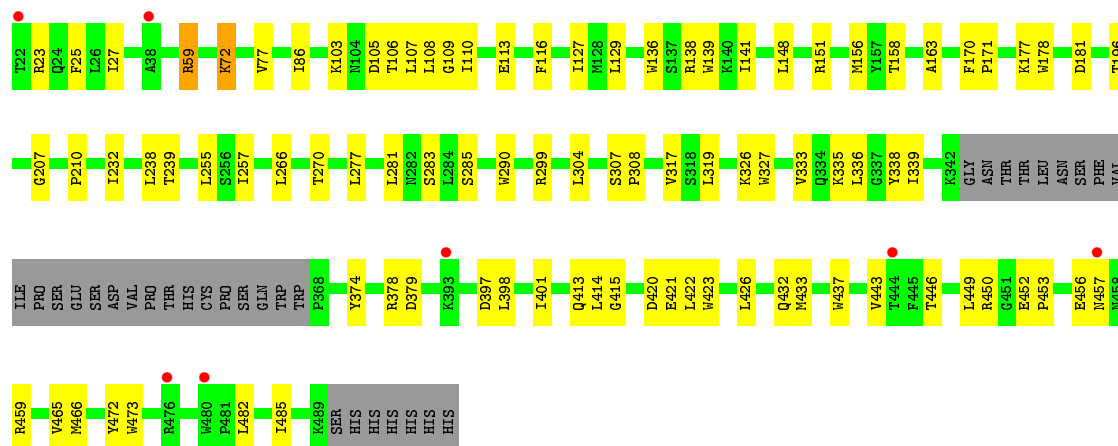
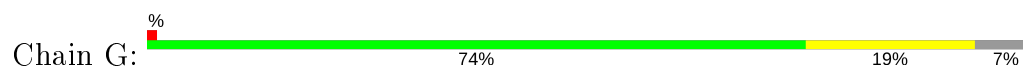




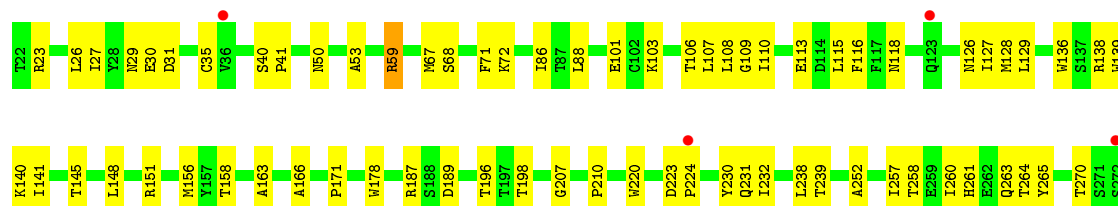
• Molecule 1: Macrophage mannose receptor 1

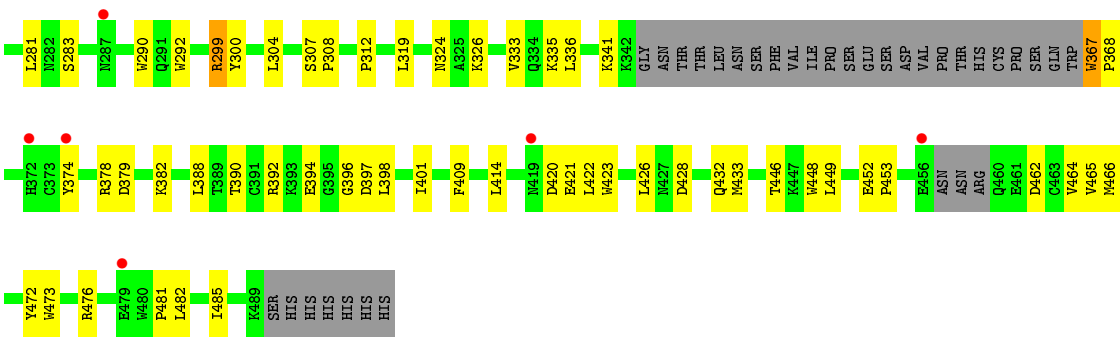


• Molecule 1: Macrophage mannose receptor 1



• Molecule 1: Macrophage mannose receptor 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	43.82Å 164.77Å 164.60Å 91.11° 97.56° 97.50°	Depositor
Resolution (Å)	27.94 – 3.20 29.90 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.1 (27.94-3.20) 92.1 (29.90-3.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 3.18Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.211 , 0.248 0.211 , 0.248	Depositor DCC
R_{free} test set	2019 reflections (2.81%)	wwPDB-VP
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.548	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , -28.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-h-l,k 0.000 for h,l,-h-k 0.406 for h,-h-k,-h-l 0.003 for -h,-k,h+l 0.005 for -h,h+k,-l 0.058 for -h,-l,-k 0.057 for -h,h+l,h+k	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	28716	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.24	0/3668	0.44	0/4968
1	B	0.24	0/3668	0.44	0/4968
1	C	0.24	0/3646	0.45	0/4938
1	D	0.24	0/3668	0.45	0/4968
1	E	0.24	0/3675	0.45	0/4978
1	F	0.24	0/3658	0.44	0/4953
1	G	0.24	0/3659	0.44	0/4954
1	H	0.24	0/3647	0.44	0/4939
All	All	0.24	0/29289	0.44	0/39666

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3570	0	3392	91	0
1	B	3570	0	3393	74	0
1	C	3549	0	3371	87	0
1	D	3570	0	3392	78	0
1	E	3577	0	3400	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3561	0	3386	71	0
1	G	3563	0	3391	63	0
1	H	3550	0	3373	101	0
2	A	12	13	13	0	0
2	B	12	13	13	0	0
2	C	12	13	13	0	0
2	D	12	13	13	0	0
2	E	12	13	13	2	0
2	F	12	13	13	0	0
2	G	12	13	13	1	0
2	H	12	13	13	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
All	All	28612	104	27202	627	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 11.

All (627) 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:D:72:LYS:NZ	1:D:178:TRP:O	2.09	0.84
1:A:264:THR:CG2	1:H:265:TYR:HB2	2.08	0.83
1:E:103:LYS:O	1:E:107:LEU:HB2	1.78	0.83
1:A:265:TYR:HB2	1:H:264:THR:CG2	2.08	0.83
1:E:422:LEU:HD12	1:E:485:ILE:HD11	1.60	0.82
1:F:141:ILE:HD13	1:F:151:ARG:HG3	1.64	0.79
1:G:374:TYR:HB2	1:G:414:LEU:HD11	1.63	0.79
1:E:378:ARG:NH1	1:E:420:ASP:OD1	2.16	0.79
1:A:141:ILE:HD13	1:A:151:ARG:HG3	1.63	0.78
1:H:103:LYS:O	1:H:107:LEU:HB2	1.83	0.78
1:D:103:LYS:O	1:D:107:LEU:HB2	1.84	0.78
1:H:382:LYS:NZ	1:H:390:THR:OG1	2.16	0.77
1:A:376:ILE:HG13	1:A:414:LEU:HD23	1.66	0.77
1:H:187:ARG:NH2	1:H:189:ASP:OD2	2.16	0.77
1:B:108:LEU:HD22	1:B:148:LEU:HD12	1.67	0.77
1:E:367:TRP:HZ2	1:E:413:GLN:HB3	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:101:GLU:OE2	1:H:103:LYS:HE3	1.86	0.75
1:A:324:ASN:HB3	1:H:224:PRO:HB2	1.66	0.75
1:C:103:LYS:O	1:C:107:LEU:HB2	1.86	0.75
1:G:103:LYS:O	1:G:107:LEU:HB2	1.86	0.75
1:E:367:TRP:CZ2	1:E:413:GLN:HB3	2.22	0.75
1:B:156:MET:HG2	1:B:210:PRO:CG	2.18	0.74
1:H:283:SER:HB3	1:H:290:TRP:CZ3	2.22	0.74
1:C:378:ARG:NH1	1:C:420:ASP:OD1	2.20	0.74
1:D:378:ARG:NH2	1:D:415:GLY:O	2.21	0.74
1:F:378:ARG:NH2	1:F:415:GLY:O	2.20	0.74
1:G:72:LYS:NZ	1:G:178:TRP:O	2.20	0.74
1:C:156:MET:HG2	1:C:210:PRO:CG	2.19	0.73
1:B:426:LEU:HD23	1:B:464:VAL:HG21	1.70	0.73
1:E:367:TRP:CD1	1:E:414:LEU:HD12	2.23	0.73
1:B:103:LYS:O	1:B:107:LEU:HB2	1.89	0.73
1:H:378:ARG:NH1	1:H:420:ASP:OD1	2.22	0.72
1:D:108:LEU:HD22	1:D:148:LEU:HD12	1.71	0.72
1:G:163:ALA:CB	1:G:196:THR:HG21	2.19	0.72
1:F:103:LYS:O	1:F:107:LEU:HB2	1.89	0.72
1:C:422:LEU:HD12	1:C:485:ILE:HD11	1.72	0.72
1:A:264:THR:HG22	1:H:265:TYR:HB2	1.70	0.72
1:A:265:TYR:HB2	1:H:264:THR:HG22	1.71	0.71
1:E:374:TYR:HB2	1:E:414:LEU:HD11	1.73	0.71
1:B:376:ILE:HG13	1:B:414:LEU:HD23	1.72	0.70
1:D:382:LYS:NZ	1:D:390:THR:OG1	2.24	0.70
1:B:422:LEU:HD12	1:B:485:ILE:HD11	1.72	0.70
1:A:103:LYS:O	1:A:107:LEU:HB2	1.92	0.70
1:C:421:GLU:HG2	1:C:482:LEU:HD13	1.74	0.70
1:A:261:HIS:O	1:H:264:THR:HG21	1.91	0.69
1:H:163:ALA:CB	1:H:196:THR:HG21	2.23	0.69
1:A:378:ARG:NH1	1:A:420:ASP:OD1	2.26	0.68
1:E:367:TRP:HD1	1:E:414:LEU:HD12	1.56	0.68
1:A:264:THR:HG21	1:H:261:HIS:O	1.92	0.68
1:A:432:GLN:HG3	1:A:433:MET:HG2	1.74	0.68
1:C:432:GLN:HG3	1:C:433:MET:HG2	1.74	0.68
1:F:432:GLN:HG3	1:F:433:MET:HG2	1.74	0.68
1:B:101:GLU:OE2	1:B:103:LYS:HE3	1.93	0.68
1:F:376:ILE:HG13	1:F:414:LEU:HD23	1.76	0.68
1:F:397:ASP:OD1	1:F:398:LEU:N	2.27	0.68
1:C:283:SER:HB3	1:C:290:TRP:CZ3	2.29	0.67
1:C:31:ASP:OD2	1:C:136:TRP:NE1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:422:LEU:HD12	1:G:485:ILE:HD11	1.74	0.67
1:E:141:ILE:HD13	1:E:151:ARG:HG3	1.76	0.67
1:G:378:ARG:NH1	1:G:420:ASP:OD1	2.27	0.67
1:B:156:MET:HG2	1:B:210:PRO:HG2	1.76	0.67
1:G:421:GLU:HG2	1:G:482:LEU:HD13	1.77	0.67
1:B:401:ILE:HD11	1:B:466:MET:HE1	1.77	0.67
1:H:108:LEU:HD22	1:H:148:LEU:HD12	1.78	0.66
1:H:72:LYS:HG2	1:H:178:TRP:HB3	1.77	0.66
1:B:378:ARG:NH1	1:B:420:ASP:OD1	2.28	0.66
1:E:77:VAL:HG12	1:E:86:ILE:HG12	1.77	0.65
1:D:101:GLU:OE2	1:D:103:LYS:HE3	1.95	0.65
1:B:421:GLU:HG2	1:B:482:LEU:HD13	1.78	0.65
1:D:232:ILE:HD13	1:D:270:THR:HG22	1.79	0.65
1:H:432:GLN:HG3	1:H:433:MET:HG2	1.77	0.64
1:B:232:ILE:HD13	1:B:270:THR:HG22	1.78	0.64
1:E:201:ASP:O	1:E:204:LYS:HE3	1.97	0.64
1:F:304:LEU:CD2	1:F:326:LYS:HB2	2.28	0.64
1:G:397:ASP:OD1	1:G:398:LEU:N	2.30	0.64
1:A:257:ILE:HG21	1:A:263:GLN:HB2	1.79	0.64
1:D:426:LEU:HD23	1:D:464:VAL:HG21	1.79	0.64
1:B:141:ILE:HD13	1:B:151:ARG:HG3	1.79	0.63
1:B:371:GLY:O	1:B:489:LYS:HD2	1.99	0.63
1:H:421:GLU:HG2	1:H:482:LEU:HD13	1.78	0.63
1:F:163:ALA:CB	1:F:196:THR:HG21	2.29	0.63
1:D:187:ARG:NH2	1:D:189:ASP:OD2	2.31	0.63
1:B:29:ASN:HB2	1:B:139:TRP:CZ3	2.34	0.63
1:F:101:GLU:OE2	1:F:103:LYS:HE3	1.98	0.63
1:C:432:GLN:HA	1:C:432:GLN:HE21	1.63	0.63
1:D:283:SER:HB3	1:D:290:TRP:CZ3	2.34	0.62
1:H:281:LEU:HB2	1:H:292:TRP:CZ3	2.35	0.62
1:E:156:MET:HG2	1:E:210:PRO:CG	2.30	0.62
1:H:465:VAL:HG11	1:H:476:ARG:HD3	1.79	0.62
1:G:141:ILE:HD13	1:G:151:ARG:HG3	1.81	0.62
1:H:141:ILE:HD13	1:H:151:ARG:HG3	1.81	0.62
1:A:397:ASP:OD1	1:A:398:LEU:N	2.33	0.62
1:C:156:MET:HG2	1:C:210:PRO:HG2	1.81	0.61
1:B:432:GLN:HG3	1:B:433:MET:HG2	1.82	0.61
1:E:397:ASP:OD1	1:E:398:LEU:N	2.32	0.61
1:H:397:ASP:OD1	1:H:398:LEU:N	2.33	0.61
1:A:101:GLU:OE2	1:A:103:LYS:HE3	2.01	0.60
1:F:72:LYS:NZ	1:F:178:TRP:O	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:397:ASP:OD1	1:B:398:LEU:N	2.34	0.60
1:F:283:SER:HB3	1:F:290:TRP:CZ3	2.35	0.60
1:G:141:ILE:CD1	1:G:151:ARG:HG3	2.31	0.60
1:A:283:SER:HB3	1:A:290:TRP:CZ3	2.36	0.60
1:E:232:ILE:HD13	1:E:270:THR:HG22	1.82	0.60
1:B:374:TYR:HB2	1:B:414:LEU:HD11	1.84	0.60
1:C:397:ASP:OD1	1:C:398:LEU:N	2.34	0.60
1:H:422:LEU:HD12	1:H:485:ILE:HD11	1.84	0.60
1:D:141:ILE:CD1	1:D:151:ARG:HG3	2.32	0.60
1:G:401:ILE:HD11	1:G:466:MET:HE1	1.83	0.59
1:A:77:VAL:HG12	1:A:86:ILE:HG12	1.84	0.59
1:E:141:ILE:CD1	1:E:151:ARG:HG3	2.31	0.59
1:F:187:ARG:NH2	1:F:189:ASP:OD2	2.32	0.59
1:A:304:LEU:CD2	1:A:326:LYS:HB2	2.32	0.59
1:F:257:ILE:HG21	1:F:263:GLN:HB2	1.84	0.59
1:H:304:LEU:HD23	1:H:326:LYS:HD2	1.84	0.59
1:H:449:LEU:CD2	1:H:472:TYR:HB2	2.32	0.59
1:A:324:ASN:HB3	1:H:224:PRO:CB	2.33	0.59
1:D:252:ALA:HB1	1:D:341:LYS:O	2.02	0.59
1:D:397:ASP:OD1	1:D:398:LEU:N	2.34	0.59
1:F:281:LEU:HB3	1:F:317:VAL:HB	1.84	0.59
1:G:452:GLU:HB3	1:G:453:PRO:HA	1.84	0.59
1:A:141:ILE:CD1	1:A:151:ARG:HG3	2.32	0.59
1:A:29:ASN:HB2	1:A:139:TRP:CZ3	2.38	0.59
1:G:25:PHE:HB2	1:G:141:ILE:HG23	1.84	0.59
1:H:239:THR:HG22	1:H:333:VAL:O	2.02	0.59
1:B:256:SER:HA	1:B:292:TRP:CE3	2.38	0.58
1:B:25:PHE:HB2	1:B:141:ILE:HG23	1.85	0.58
1:E:108:LEU:HD22	1:E:148:LEU:HD12	1.84	0.58
1:E:304:LEU:CD2	1:E:326:LYS:HB2	2.34	0.58
1:A:158:THR:HB	1:A:207:GLY:HA3	1.85	0.58
1:D:141:ILE:HD13	1:D:151:ARG:HG3	1.85	0.58
1:B:75:LEU:HD23	1:B:88:LEU:HD23	1.84	0.58
1:B:238:LEU:HD12	1:B:338:TYR:CE2	2.39	0.58
1:C:378:ARG:NH2	1:C:420:ASP:OD2	2.36	0.58
1:A:376:ILE:CG1	1:A:414:LEU:HD23	2.35	0.57
1:G:156:MET:HG2	1:G:210:PRO:CG	2.34	0.57
1:C:187:ARG:NH2	1:C:189:ASP:OD2	2.36	0.57
1:G:108:LEU:HD22	1:G:148:LEU:HD12	1.86	0.57
1:H:141:ILE:CD1	1:H:151:ARG:HG3	2.34	0.57
1:E:156:MET:HG2	1:E:210:PRO:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:281:LEU:HB3	1:G:317:VAL:HB	1.85	0.57
1:H:86:ILE:HD12	1:H:127:ILE:HG22	1.87	0.57
1:B:378:ARG:NH2	1:B:415:GLY:O	2.36	0.57
1:H:283:SER:HB3	1:H:290:TRP:CE3	2.39	0.57
1:D:379:ASP:N	1:D:379:ASP:OD1	2.38	0.57
1:F:108:LEU:HD22	1:F:148:LEU:HD12	1.86	0.57
1:C:101:GLU:OE2	1:C:103:LYS:HE3	2.06	0.56
1:G:27:ILE:HG22	1:G:139:TRP:CE3	2.39	0.56
1:F:110:ILE:CG2	1:F:113:GLU:HB2	2.35	0.56
1:F:379:ASP:N	1:F:379:ASP:OD1	2.38	0.56
1:F:72:LYS:N	1:F:72:LYS:HD2	2.20	0.56
1:D:117:PHE:CZ	1:D:127:ILE:HG21	2.40	0.56
1:D:158:THR:HG23	1:D:166:ALA:O	2.05	0.56
1:E:106:THR:HB	1:E:138:ARG:HB3	1.87	0.56
1:E:257:ILE:HD12	1:E:327:TRP:CZ2	2.41	0.56
1:A:371:GLY:O	1:A:489:LYS:HD2	2.05	0.56
1:G:238:LEU:HD12	1:G:338:TYR:CE2	2.40	0.56
1:G:285:SER:O	1:G:450:ARG:NH1	2.37	0.56
1:D:163:ALA:CB	1:D:196:THR:HG21	2.35	0.56
1:B:40:SER:HA	1:B:71:PHE:CE2	2.41	0.56
1:E:158:THR:HB	1:E:207:GLY:HA3	1.88	0.56
1:C:371:GLY:O	1:C:489:LYS:HD2	2.06	0.56
1:D:421:GLU:HG2	1:D:482:LEU:HD13	1.88	0.56
1:F:25:PHE:HB2	1:F:141:ILE:HG23	1.88	0.56
1:F:77:VAL:HG12	1:F:86:ILE:HG12	1.88	0.56
1:D:388:LEU:HD13	1:D:398:LEU:HD12	1.88	0.56
1:H:163:ALA:HB1	1:H:196:THR:HG21	1.88	0.56
1:B:304:LEU:CD2	1:B:326:LYS:HB2	2.36	0.56
1:H:392:ARG:HA	1:H:396:GLY:O	2.05	0.56
1:B:379:ASP:OD1	1:B:379:ASP:N	2.39	0.56
1:A:267:THR:HG22	1:H:265:TYR:HE2	1.71	0.56
1:H:50:ASN:ND2	1:H:53:ALA:HB2	2.21	0.56
1:C:281:LEU:HB3	1:C:317:VAL:HB	1.88	0.55
1:E:421:GLU:HG2	1:E:482:LEU:HD13	1.88	0.55
1:A:279:ILE:HD11	1:A:317:VAL:HG12	1.89	0.55
1:A:281:LEU:HB3	1:A:317:VAL:HB	1.88	0.55
1:E:369:TYR:HB2	1:E:409:PHE:CE1	2.42	0.55
1:B:460:GLN:O	1:B:462:ASP:N	2.40	0.55
1:C:108:LEU:HD22	1:C:148:LEU:HD12	1.89	0.55
1:C:158:THR:HB	1:C:207:GLY:HA3	1.88	0.55
1:A:108:LEU:HD22	1:A:148:LEU:HD12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LYS:HD2	1:A:72:LYS:N	2.21	0.55
1:B:257:ILE:HG21	1:B:263:GLN:HB2	1.89	0.55
1:B:28:TYR:CE2	1:B:30:GLU:HA	2.42	0.55
1:C:260:ILE:HG12	1:C:300:TYR:CE1	2.42	0.55
1:H:110:ILE:CG2	1:H:113:GLU:HB2	2.37	0.55
1:C:115:LEU:HB3	1:C:129:LEU:HG	1.89	0.55
1:C:426:LEU:HD23	1:C:464:VAL:HG21	1.89	0.55
1:E:72:LYS:N	1:E:72:LYS:HD2	2.22	0.55
1:D:422:LEU:HD12	1:D:485:ILE:HD11	1.89	0.55
1:G:106:THR:HB	1:G:138:ARG:HB3	1.89	0.55
1:A:379:ASP:N	1:A:379:ASP:OD1	2.40	0.55
1:C:70:ALA:O	1:D:41:PRO:HG2	2.07	0.54
1:B:252:ALA:HB1	1:B:341:LYS:O	2.06	0.54
1:C:29:ASN:HB2	1:C:139:TRP:CZ3	2.43	0.54
1:C:72:LYS:HG2	1:C:178:TRP:HB3	1.88	0.54
1:F:28:TYR:CE2	1:F:30:GLU:HA	2.43	0.54
1:D:335:LYS:O	1:D:336:LEU:HD23	2.07	0.54
1:C:239:THR:HG22	1:C:333:VAL:O	2.08	0.54
1:C:177:LYS:HD3	1:D:89:TYR:CD2	2.43	0.54
1:H:23:ARG:HE	1:H:59:ARG:NH2	2.05	0.54
1:B:281:LEU:HB3	1:B:317:VAL:HB	1.90	0.54
1:C:401:ILE:HD11	1:C:466:MET:HE1	1.89	0.54
1:D:156:MET:HG2	1:D:210:PRO:CG	2.38	0.54
1:E:163:ALA:CB	1:E:196:THR:HG21	2.38	0.54
1:G:335:LYS:O	1:G:336:LEU:HD23	2.07	0.54
1:G:283:SER:HB3	1:G:290:TRP:CZ3	2.43	0.54
1:G:72:LYS:N	1:G:72:LYS:HD2	2.23	0.54
1:B:374:TYR:HB2	1:B:414:LEU:CD1	2.38	0.53
1:B:303:TRP:CD2	1:B:308:PRO:HD3	2.43	0.53
1:C:141:ILE:HD13	1:C:151:ARG:HG3	1.90	0.53
1:C:455:HIS:ND1	1:C:461:GLU:O	2.39	0.53
1:D:29:ASN:HB2	1:D:139:TRP:CZ3	2.43	0.53
1:D:72:LYS:HD2	1:D:72:LYS:N	2.22	0.53
1:B:72:LYS:N	1:B:72:LYS:HD2	2.24	0.53
1:E:106:THR:CB	1:E:138:ARG:HB3	2.38	0.53
1:F:378:ARG:NH1	1:F:420:ASP:OD1	2.42	0.53
1:E:72:LYS:NZ	1:E:178:TRP:O	2.35	0.53
1:H:304:LEU:CD2	1:H:326:LYS:HB2	2.39	0.53
1:D:460:GLN:O	1:D:462:ASP:N	2.42	0.53
1:E:103:LYS:NZ	1:E:113:GLU:O	2.39	0.53
1:G:304:LEU:HD23	1:G:326:LYS:HD2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:379:ASP:OD1	1:G:379:ASP:N	2.41	0.53
1:H:379:ASP:N	1:H:379:ASP:OD1	2.42	0.53
1:H:448:TRP:CZ3	1:H:453:PRO:HB3	2.44	0.53
1:A:447:LYS:HD2	1:A:472:TYR:CE1	2.44	0.53
1:B:257:ILE:HD12	1:B:327:TRP:CZ2	2.43	0.53
1:C:379:ASP:OD1	1:C:379:ASP:N	2.42	0.53
1:C:77:VAL:HG12	1:C:86:ILE:HG12	1.91	0.53
1:G:23:ARG:HE	1:G:59:ARG:NH2	2.07	0.53
1:C:163:ALA:CB	1:C:196:THR:HG21	2.38	0.53
1:C:367:TRP:CG	1:H:312:PRO:HG2	2.43	0.53
1:C:392:ARG:HA	1:C:396:GLY:O	2.08	0.53
1:E:303:TRP:CD2	1:E:308:PRO:HD3	2.43	0.53
1:C:367:TRP:CD1	1:H:312:PRO:HG2	2.44	0.53
1:A:156:MET:HG2	1:A:210:PRO:CG	2.38	0.53
1:C:376:ILE:HG13	1:C:414:LEU:HD23	1.91	0.53
1:A:158:THR:HG23	1:A:166:ALA:O	2.10	0.52
1:D:448:TRP:CD2	1:D:453:PRO:HD3	2.44	0.52
1:B:448:TRP:CG	1:B:453:PRO:HD3	2.42	0.52
1:F:141:ILE:CD1	1:F:151:ARG:HG3	2.38	0.52
1:C:72:LYS:HD2	1:C:72:LYS:N	2.25	0.52
1:F:257:ILE:HD13	1:F:263:GLN:OE1	2.09	0.52
1:A:376:ILE:HG13	1:A:414:LEU:CD2	2.38	0.52
1:E:374:TYR:CB	1:E:414:LEU:HD11	2.38	0.52
1:G:432:GLN:HG3	1:G:433:MET:HG2	1.91	0.52
1:F:75:LEU:HD23	1:F:88:LEU:HD23	1.91	0.52
1:A:422:LEU:HD12	1:A:485:ILE:HD11	1.92	0.52
1:F:421:GLU:HG2	1:F:482:LEU:HD13	1.92	0.52
1:B:256:SER:HA	1:B:292:TRP:CZ3	2.45	0.52
1:H:115:LEU:HB3	1:H:129:LEU:HG	1.91	0.52
1:F:335:LYS:O	1:F:336:LEU:HD23	2.09	0.52
1:A:448:TRP:CD2	1:A:453:PRO:HD3	2.45	0.52
1:C:426:LEU:HB2	1:C:437:TRP:CZ3	2.45	0.52
1:G:86:ILE:HD12	1:G:127:ILE:HG22	1.91	0.51
1:F:426:LEU:HB2	1:F:437:TRP:CZ3	2.46	0.51
1:A:28:TYR:CE2	1:A:30:GLU:HA	2.45	0.51
1:F:158:THR:HG23	1:F:166:ALA:O	2.10	0.51
1:F:448:TRP:CD2	1:F:453:PRO:HD3	2.45	0.51
1:C:126:ASN:ND2	1:C:127:ILE:O	2.43	0.51
1:E:376:ILE:HG13	1:E:414:LEU:HD23	1.93	0.51
1:E:77:VAL:CG1	1:E:86:ILE:HG12	2.39	0.51
1:H:30:GLU:OE2	1:H:140:LYS:HD2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:MET:HG2	1:D:210:PRO:HG2	1.93	0.51
1:E:379:ASP:N	1:E:379:ASP:OD1	2.43	0.51
1:A:279:ILE:HD11	1:A:317:VAL:CG1	2.40	0.51
1:D:41:PRO:HD3	1:D:71:PHE:CE2	2.45	0.51
1:A:156:MET:HG2	1:A:210:PRO:HD2	1.93	0.51
1:A:307:SER:HA	1:A:308:PRO:C	2.31	0.51
1:E:432:GLN:HG3	1:E:433:MET:HG2	1.92	0.51
1:A:264:THR:HG22	1:H:265:TYR:CB	2.39	0.51
1:E:281:LEU:HB3	1:E:317:VAL:HB	1.91	0.51
1:F:260:ILE:HG12	1:F:300:TYR:CE1	2.46	0.51
1:H:27:ILE:HG22	1:H:139:TRP:CE3	2.46	0.51
1:H:31:ASP:OD2	1:H:136:TRP:NE1	2.41	0.50
1:A:110:ILE:CG2	1:A:113:GLU:HB2	2.41	0.50
1:D:59:ARG:HG2	1:D:60:TRP:N	2.25	0.50
1:E:376:ILE:CG1	1:E:414:LEU:HD23	2.40	0.50
1:A:187:ARG:NH2	1:A:189:ASP:OD2	2.40	0.50
1:C:367:TRP:CD1	1:C:367:TRP:N	2.80	0.50
1:C:75:LEU:HD23	1:C:88:LEU:HD23	1.92	0.50
1:D:238:LEU:HD12	1:D:338:TYR:CE2	2.46	0.50
1:D:40:SER:HA	1:D:71:PHE:CE2	2.47	0.50
1:B:304:LEU:HD23	1:B:326:LYS:HD2	1.93	0.50
1:B:163:ALA:CB	1:B:196:THR:HG21	2.41	0.50
1:B:40:SER:HA	1:B:71:PHE:HE2	1.75	0.50
1:C:23:ARG:HE	1:C:59:ARG:NH2	2.09	0.50
1:D:281:LEU:HB3	1:D:317:VAL:HB	1.94	0.50
1:H:223:ASP:HB2	1:H:230:TYR:HE2	1.77	0.50
1:H:260:ILE:HG12	1:H:300:TYR:CE1	2.46	0.50
1:A:126:ASN:ND2	1:A:127:ILE:O	2.45	0.50
1:B:283:SER:HB3	1:B:290:TRP:CZ3	2.46	0.50
1:A:265:TYR:CB	1:H:264:THR:HG22	2.42	0.50
1:C:119:TYR:HB2	1:C:127:ILE:HD13	1.92	0.50
1:H:252:ALA:HB1	1:H:341:LYS:O	2.12	0.50
1:H:446:THR:HA	1:H:473:TRP:CZ3	2.47	0.50
1:B:307:SER:HA	1:B:308:PRO:C	2.32	0.49
1:E:465:VAL:HG11	1:E:476:ARG:HD3	1.94	0.49
1:H:374:TYR:HB2	1:H:414:LEU:HD11	1.94	0.49
1:A:264:THR:HG21	1:H:265:TYR:HB2	1.89	0.49
1:B:108:LEU:CD2	1:B:148:LEU:HD12	2.38	0.49
1:C:283:SER:HB3	1:C:290:TRP:CE3	2.47	0.49
1:A:228:VAL:HG11	1:A:341:LYS:HE3	1.95	0.49
1:B:59:ARG:HG2	1:B:60:TRP:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:77:VAL:CG1	1:F:86:ILE:HG12	2.43	0.49
1:G:304:LEU:CD2	1:G:326:LYS:HB2	2.41	0.49
1:D:382:LYS:O	1:D:481:PRO:HA	2.13	0.49
1:D:283:SER:HB3	1:D:290:TRP:CE3	2.47	0.49
1:D:28:TYR:CE2	1:D:30:GLU:HA	2.47	0.49
1:E:335:LYS:O	1:E:336:LEU:HD23	2.12	0.49
1:C:304:LEU:CD2	1:C:326:LYS:HB2	2.41	0.49
1:C:335:LYS:O	1:C:336:LEU:HD23	2.13	0.49
1:E:23:ARG:HE	1:E:59:ARG:NH2	2.11	0.49
1:F:276:GLY:O	1:F:277:LEU:HD23	2.13	0.49
1:F:392:ARG:HA	1:F:396:GLY:O	2.11	0.49
1:G:106:THR:OG1	1:G:138:ARG:HD3	2.12	0.49
1:A:455:HIS:ND1	1:A:461:GLU:O	2.45	0.49
1:E:27:ILE:HG22	1:E:139:TRP:CE3	2.47	0.49
1:E:29:ASN:HB2	1:E:139:TRP:CZ3	2.48	0.49
1:F:252:ALA:HB1	1:F:341:LYS:O	2.12	0.49
1:C:256:SER:HA	1:C:292:TRP:CE3	2.47	0.49
1:F:258:THR:O	1:F:299:ARG:HD2	2.12	0.49
1:B:452:GLU:HB3	1:B:453:PRO:HA	1.95	0.48
1:F:80:LYS:HD3	1:F:113:GLU:HG3	1.94	0.48
1:H:72:LYS:N	1:H:72:LYS:HD2	2.28	0.48
1:B:158:THR:HB	1:B:207:GLY:HA3	1.95	0.48
1:C:309:SER:OG	1:C:314:LYS:HD2	2.13	0.48
1:D:432:GLN:HG3	1:D:433:MET:HG2	1.94	0.48
1:G:449:LEU:CD2	1:G:472:TYR:HB2	2.43	0.48
1:A:107:LEU:HD23	1:A:138:ARG:HG2	1.95	0.48
1:A:465:VAL:HG11	1:A:476:ARG:HD3	1.95	0.48
1:D:40:SER:HA	1:D:71:PHE:HE2	1.79	0.48
1:A:265:TYR:HB2	1:H:264:THR:HG21	1.92	0.48
1:B:376:ILE:CG1	1:B:414:LEU:HD23	2.43	0.48
1:C:41:PRO:HD3	1:C:71:PHE:CE2	2.49	0.48
1:A:201:ASP:O	1:A:204:LYS:HE3	2.12	0.48
1:E:25:PHE:HB2	1:E:141:ILE:HG23	1.94	0.48
1:F:238:LEU:O	1:F:335:LYS:HA	2.13	0.48
1:H:238:LEU:O	1:H:335:LYS:HA	2.13	0.48
1:H:367:TRP:CE3	1:H:368:PRO:HD2	2.48	0.48
1:D:374:TYR:HB2	1:D:414:LEU:HD11	1.94	0.48
1:E:304:LEU:HD23	1:E:326:LYS:HB2	1.94	0.48
1:G:156:MET:HG2	1:G:210:PRO:HG2	1.95	0.48
1:A:109:GLY:HA2	1:A:116:PHE:HA	1.95	0.48
1:C:27:ILE:HG22	1:C:139:TRP:CE3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:388:LEU:HD13	1:C:398:LEU:HD12	1.96	0.48
1:D:257:ILE:HG21	1:D:263:GLN:HB2	1.96	0.48
1:H:220:TRP:CE3	1:H:231:GLN:HB2	2.48	0.48
1:B:448:TRP:CD2	1:B:453:PRO:HD3	2.49	0.48
1:E:23:ARG:NH2	1:E:181:ASP:OD2	2.46	0.48
1:F:126:ASN:ND2	1:F:127:ILE:O	2.47	0.48
1:F:367:TRP:O	1:F:373:CYS:HA	2.13	0.48
1:G:437:TRP:CD1	1:G:443:VAL:HG22	2.49	0.48
1:H:401:ILE:HD11	1:H:466:MET:HE1	1.96	0.48
1:A:75:LEU:HD23	1:A:88:LEU:HD23	1.96	0.47
1:A:77:VAL:CG1	1:A:86:ILE:HG12	2.44	0.47
1:G:77:VAL:HG12	1:G:86:ILE:HG12	1.97	0.47
1:D:448:TRP:CZ3	1:D:453:PRO:HB3	2.50	0.47
1:F:307:SER:HA	1:F:308:PRO:C	2.35	0.47
1:C:77:VAL:CG1	1:C:86:ILE:HG12	2.43	0.47
1:A:117:PHE:CZ	1:A:127:ILE:HG21	2.49	0.47
1:G:108:LEU:CD2	1:G:148:LEU:HD12	2.44	0.47
1:G:232:ILE:HD13	1:G:270:THR:HG22	1.96	0.47
1:H:307:SER:HA	1:H:308:PRO:C	2.34	0.47
1:F:158:THR:HB	1:F:207:GLY:HA3	1.96	0.47
1:A:156:MET:HG2	1:A:210:PRO:HG2	1.96	0.47
1:C:314:LYS:HD3	1:C:329:ASN:O	2.15	0.47
1:E:238:LEU:HD12	1:E:338:TYR:CE2	2.49	0.47
1:E:452:GLU:HB3	1:E:453:PRO:HA	1.96	0.47
1:G:136:TRP:HB2	2:G:501:MES:O2S	2.14	0.47
1:E:134:GLY:HA3	2:E:501:MES:H82	1.97	0.47
1:F:239:THR:HG22	1:F:333:VAL:O	2.15	0.47
1:G:257:ILE:HD12	1:G:327:TRP:CZ2	2.50	0.47
1:H:319:LEU:HD23	1:H:319:LEU:C	2.35	0.47
1:B:141:ILE:CD1	1:B:151:ARG:HG3	2.43	0.47
1:E:106:THR:OG1	1:E:138:ARG:HB3	2.14	0.47
1:E:99:LYS:HD3	1:E:111:LYS:HE3	1.96	0.47
1:H:106:THR:OG1	1:H:138:ARG:HB3	2.15	0.47
1:H:367:TRP:HE3	1:H:368:PRO:HD2	1.80	0.47
1:H:423:TRP:CE3	1:H:465:VAL:HG12	2.50	0.47
1:D:281:LEU:HD23	1:D:317:VAL:HG11	1.97	0.46
1:H:126:ASN:ND2	1:H:127:ILE:O	2.47	0.46
1:A:335:LYS:O	1:A:336:LEU:HD23	2.15	0.46
1:B:424:ILE:HD11	1:B:464:VAL:HG12	1.96	0.46
1:D:452:GLU:HB3	1:D:453:PRO:HA	1.97	0.46
1:E:281:LEU:HB2	1:E:292:TRP:CZ3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:158:THR:HB	1:G:207:GLY:HA3	1.97	0.46
1:G:319:LEU:C	1:G:319:LEU:HD23	2.36	0.46
1:F:107:LEU:HD23	1:F:138:ARG:HG2	1.96	0.46
1:H:158:THR:HB	1:H:207:GLY:HA3	1.96	0.46
1:A:239:THR:HG22	1:A:333:VAL:O	2.15	0.46
1:A:376:ILE:HG12	1:A:485:ILE:HG12	1.98	0.46
1:B:201:ASP:O	1:B:204:LYS:HE3	2.16	0.46
1:E:115:LEU:HB3	1:E:129:LEU:HG	1.96	0.46
1:H:118:ASN:HB3	1:H:128:MET:O	2.16	0.46
1:H:156:MET:HG2	1:H:210:PRO:HG2	1.97	0.46
1:H:388:LEU:HD11	1:H:397:ASP:OD1	2.16	0.46
1:C:72:LYS:HE3	1:C:178:TRP:O	2.16	0.46
1:D:463:CYS:O	1:D:475:ASP:HA	2.15	0.46
1:E:372:HIS:CD2	1:E:487:LYS:HE2	2.50	0.46
1:H:258:THR:O	1:H:299:ARG:HD2	2.15	0.46
1:F:281:LEU:HD23	1:F:317:VAL:HG11	1.97	0.46
1:F:384:GLN:HG3	1:F:463:CYS:SG	2.56	0.46
1:C:465:VAL:HG11	1:C:476:ARG:HD3	1.97	0.46
1:A:234:SER:HB3	1:A:273:LEU:HD13	1.97	0.46
1:D:86:ILE:HD12	1:D:127:ILE:HG22	1.98	0.46
1:E:390:THR:O	1:E:394:GLU:HG3	2.15	0.46
1:A:426:LEU:HB2	1:A:437:TRP:CZ3	2.51	0.45
1:C:448:TRP:CD2	1:C:453:PRO:HD3	2.51	0.45
1:D:382:LYS:C	1:D:481:PRO:HA	2.36	0.45
1:F:156:MET:HG2	1:F:210:PRO:CG	2.45	0.45
1:F:319:LEU:HD23	1:F:319:LEU:C	2.35	0.45
1:C:41:PRO:HD3	1:C:71:PHE:CD2	2.51	0.45
1:E:109:GLY:HA2	1:E:116:PHE:HA	1.98	0.45
1:F:231:GLN:HB3	1:F:340:CYS:HB2	1.98	0.45
1:F:452:GLU:HB3	1:F:453:PRO:HA	1.98	0.45
1:G:401:ILE:CD1	1:G:466:MET:HE1	2.46	0.45
1:C:367:TRP:N	1:C:368:PRO:HD3	2.32	0.45
1:C:424:ILE:HG21	1:C:466:MET:HE3	1.97	0.45
1:E:276:GLY:O	1:E:277:LEU:HD23	2.17	0.45
1:H:109:GLY:HA2	1:H:116:PHE:HA	1.98	0.45
1:A:392:ARG:HA	1:A:396:GLY:O	2.15	0.45
1:C:452:GLU:HB3	1:C:453:PRO:HA	1.97	0.45
1:E:299:ARG:HB3	1:E:443:VAL:HG11	1.99	0.45
1:F:448:TRP:CZ3	1:F:453:PRO:HB3	2.51	0.45
1:H:72:LYS:HG2	1:H:178:TRP:CB	2.45	0.45
1:B:117:PHE:CZ	1:B:127:ILE:HG21	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:MET:HG2	1:B:210:PRO:CD	2.46	0.45
1:D:401:ILE:HD11	1:D:466:MET:HE1	1.98	0.45
1:G:110:ILE:CG2	1:G:113:GLU:HB2	2.47	0.45
1:G:446:THR:HA	1:G:473:TRP:CZ3	2.51	0.45
1:C:106:THR:HB	1:C:138:ARG:HB3	1.98	0.45
1:E:303:TRP:CE2	1:E:308:PRO:HD3	2.52	0.45
1:G:163:ALA:HB1	1:G:196:THR:HG21	1.95	0.45
1:B:232:ILE:CD1	1:B:269:LEU:HB3	2.47	0.45
1:C:319:LEU:HD23	1:C:319:LEU:C	2.37	0.45
1:E:311:GLU:HA	1:E:312:PRO:HD3	1.88	0.45
1:E:319:LEU:C	1:E:319:LEU:HD23	2.38	0.45
1:F:80:LYS:HD3	1:F:113:GLU:CG	2.46	0.45
1:F:163:ALA:HB1	1:F:196:THR:HG21	1.99	0.45
1:F:257:ILE:HD12	1:F:327:TRP:CZ2	2.52	0.45
1:C:50:ASN:ND2	1:C:53:ALA:HB2	2.32	0.44
1:C:177:LYS:HD3	1:D:89:TYR:CE2	2.52	0.44
1:E:281:LEU:HD12	1:E:291:GLN:O	2.18	0.44
1:E:134:GLY:N	2:E:501:MES:O2S	2.47	0.44
1:C:257:ILE:HG21	1:C:263:GLN:HB2	1.99	0.44
1:D:108:LEU:HD22	1:D:148:LEU:CD1	2.43	0.44
1:D:158:THR:HB	1:D:207:GLY:HA3	1.98	0.44
1:D:277:LEU:HD12	1:D:339:ILE:HD11	1.99	0.44
1:F:41:PRO:HA	1:F:88:LEU:HB2	1.98	0.44
1:G:456:GLU:HB2	1:G:459:ARG:CG	2.47	0.44
1:H:390:THR:O	1:H:394:GLU:HG3	2.17	0.44
1:A:423:TRP:CE3	1:A:465:VAL:HG12	2.52	0.44
1:B:281:LEU:HD23	1:B:317:VAL:HG21	1.99	0.44
1:E:279:ILE:HD11	1:E:317:VAL:HG12	1.99	0.44
1:F:390:THR:O	1:F:394:GLU:HG3	2.17	0.44
1:G:23:ARG:NH2	1:G:181:ASP:OD2	2.50	0.44
1:G:378:ARG:NH2	1:G:415:GLY:O	2.50	0.44
1:A:224:PRO:HB3	1:H:324:ASN:OD1	2.17	0.44
1:C:277:LEU:HD12	1:C:339:ILE:HD11	1.99	0.44
1:D:307:SER:HA	1:D:308:PRO:C	2.36	0.44
1:D:64:SER:HB3	1:D:99:LYS:HB3	2.00	0.44
1:G:307:SER:HA	1:G:308:PRO:C	2.38	0.44
1:A:450:ARG:HG3	1:G:413:GLN:OE1	2.18	0.44
1:H:257:ILE:HG21	1:H:263:GLN:HB2	1.99	0.44
1:A:156:MET:HG2	1:A:210:PRO:CD	2.48	0.44
1:B:335:LYS:O	1:B:336:LEU:HD23	2.17	0.44
1:D:232:ILE:CD1	1:D:269:LEU:HB3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:ILE:CG2	1:E:113:GLU:HB2	2.48	0.44
1:H:382:LYS:O	1:H:481:PRO:HA	2.18	0.44
1:H:448:TRP:CD2	1:H:453:PRO:HD3	2.53	0.44
1:A:257:ILE:HD13	1:A:263:GLN:OE1	2.18	0.44
1:B:160:LEU:HD11	1:B:219:LEU:CD2	2.48	0.44
1:C:284:LEU:HD23	1:C:315:SER:HB3	1.98	0.44
1:D:27:ILE:HG22	1:D:139:TRP:CE3	2.53	0.44
1:D:319:LEU:C	1:D:319:LEU:HD23	2.38	0.44
1:D:387:ALA:HB1	1:D:484:TYR:CG	2.53	0.44
1:B:106:THR:OG1	1:B:138:ARG:HB3	2.17	0.44
1:C:307:SER:HA	1:C:308:PRO:C	2.37	0.44
1:C:449:LEU:CD2	1:C:472:TYR:HB2	2.48	0.44
1:D:300:TYR:C	1:D:301:LEU:HD12	2.38	0.44
1:D:41:PRO:HD3	1:D:71:PHE:CD2	2.53	0.44
1:H:72:LYS:HE3	1:H:178:TRP:O	2.18	0.44
1:H:426:LEU:HD23	1:H:464:VAL:HG21	2.00	0.44
1:A:374:TYR:HB2	1:A:414:LEU:HD11	1.99	0.44
1:E:387:ALA:HB1	1:E:484:TYR:CG	2.53	0.44
1:F:424:ILE:HD11	1:F:464:VAL:CG1	2.48	0.44
1:C:106:THR:CB	1:C:138:ARG:HB3	2.48	0.43
1:C:67:MET:HG2	1:C:68:SER:N	2.33	0.43
1:D:426:LEU:HB3	1:D:464:VAL:HB	1.99	0.43
1:H:140:LYS:HD3	1:H:145:THR:HA	2.00	0.43
1:H:428:ASP:OD1	1:H:462:ASP:HA	2.18	0.43
1:A:25:PHE:HB2	1:A:141:ILE:HG23	1.99	0.43
1:A:452:GLU:HB3	1:A:453:PRO:HA	2.00	0.43
1:G:277:LEU:HD12	1:G:339:ILE:HD11	1.99	0.43
1:H:156:MET:HG2	1:H:210:PRO:CG	2.47	0.43
1:H:452:GLU:HB3	1:H:453:PRO:HA	2.00	0.43
1:C:141:ILE:CD1	1:C:151:ARG:HG3	2.48	0.43
1:D:163:ALA:HB1	1:D:196:THR:HG21	1.97	0.43
1:G:77:VAL:HG11	1:G:129:LEU:HD22	1.99	0.43
1:B:426:LEU:HB3	1:B:464:VAL:HB	1.99	0.43
1:C:45:GLN:NE2	1:C:125:LYS:HE2	2.33	0.43
1:F:283:SER:HB3	1:F:290:TRP:CE3	2.54	0.43
1:G:106:THR:CB	1:G:138:ARG:HB3	2.46	0.43
1:H:26:LEU:HD21	1:H:50:ASN:O	2.18	0.43
1:G:255:LEU:HD21	1:G:266:LEU:HG	2.00	0.43
1:B:401:ILE:HD11	1:B:466:MET:CE	2.48	0.43
1:G:25:PHE:CE1	1:G:148:LEU:HD22	2.54	0.43
1:E:156:MET:HG2	1:E:210:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:374:TYR:HB2	1:E:414:LEU:CD1	2.45	0.43
1:G:170:PHE:HA	1:G:171:PRO:HA	1.82	0.43
1:H:409:PHE:CE2	1:H:414:LEU:HD13	2.54	0.43
1:H:41:PRO:HA	1:H:88:LEU:HB2	1.99	0.43
1:A:32:HIS:O	1:A:33:LYS:HB2	2.19	0.43
1:B:232:ILE:HD11	1:B:269:LEU:HB3	2.00	0.43
1:B:314:LYS:HD3	1:B:329:ASN:O	2.19	0.43
1:B:376:ILE:HG13	1:B:414:LEU:CD2	2.46	0.43
1:C:220:TRP:CE3	1:C:231:GLN:HB2	2.54	0.43
1:C:220:TRP:CD2	1:C:231:GLN:HB2	2.54	0.43
1:A:67:MET:CE	1:A:180:ALA:HB1	2.49	0.43
1:F:67:MET:CE	1:F:180:ALA:HB1	2.49	0.43
1:G:107:LEU:HD23	1:G:138:ARG:HG2	2.01	0.43
1:G:449:LEU:HD23	1:G:472:TYR:HB2	2.01	0.43
1:A:163:ALA:CB	1:A:196:THR:HG21	2.49	0.43
1:G:109:GLY:HA2	1:G:116:PHE:HA	2.00	0.43
1:F:460:GLN:O	1:F:462:ASP:N	2.51	0.42
1:H:158:THR:HG23	1:H:166:ALA:O	2.18	0.42
1:A:426:LEU:HD23	1:A:464:VAL:HG21	2.01	0.42
1:A:421:GLU:HG2	1:A:482:LEU:HD13	2.00	0.42
1:B:77:VAL:HG12	1:B:86:ILE:HG12	2.00	0.42
1:E:447:LYS:HD2	1:E:472:TYR:CE1	2.54	0.42
1:F:108:LEU:CD2	1:F:148:LEU:HD12	2.49	0.42
1:A:304:LEU:HD23	1:A:326:LYS:HB2	2.00	0.42
1:B:319:LEU:HD23	1:B:319:LEU:C	2.40	0.42
1:B:319:LEU:O	1:B:321:PRO:HD3	2.18	0.42
1:B:86:ILE:HD12	1:B:127:ILE:HG22	2.01	0.42
1:D:108:LEU:CD2	1:D:148:LEU:HD12	2.44	0.42
1:E:423:TRP:CE3	1:E:465:VAL:HG12	2.54	0.42
1:A:319:LEU:C	1:A:319:LEU:HD23	2.40	0.42
1:D:304:LEU:CD2	1:D:326:LYS:HB2	2.49	0.42
1:F:428:ASP:OD1	1:F:462:ASP:HA	2.19	0.42
1:E:89:TYR:CD2	1:G:177:LYS:HD3	2.55	0.42
1:A:260:ILE:HG22	1:H:261:HIS:CB	2.49	0.42
1:H:335:LYS:O	1:H:336:LEU:HD23	2.20	0.42
1:C:106:THR:OG1	1:C:138:ARG:HB3	2.19	0.42
1:C:374:TYR:HB2	1:C:414:LEU:HD11	2.02	0.42
1:D:67:MET:CE	1:D:180:ALA:HB1	2.50	0.42
1:E:23:ARG:HE	1:E:59:ARG:HH21	1.67	0.42
1:F:424:ILE:HD11	1:F:464:VAL:HG12	2.00	0.42
1:G:239:THR:HG22	1:G:333:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:MET:HE1	1:A:180:ALA:HB1	2.02	0.42
1:B:452:GLU:HG3	1:B:474:ALA:HB2	2.01	0.42
1:F:86:ILE:HD13	1:F:100:TRP:CH2	2.55	0.42
1:H:232:ILE:HD13	1:H:270:THR:HG22	2.01	0.42
1:H:40:SER:HB2	1:H:41:PRO:HD2	2.00	0.42
1:C:163:ALA:HB1	1:C:196:THR:HG21	2.02	0.42
1:D:50:ASN:ND2	1:D:53:ALA:HB2	2.35	0.42
1:E:170:PHE:HA	1:E:171:PRO:HA	1.84	0.42
1:F:304:LEU:HD23	1:F:326:LYS:HD2	2.01	0.42
1:H:388:LEU:HD13	1:H:398:LEU:HD12	2.01	0.42
1:A:304:LEU:HD12	1:A:328:GLU:HB3	2.02	0.41
1:C:304:LEU:HD23	1:C:326:LYS:HD2	2.01	0.41
1:D:106:THR:OG1	1:D:138:ARG:HB3	2.20	0.41
1:D:193:TRP:HA	1:D:208:TYR:HA	2.02	0.41
1:E:400:SER:HA	1:E:437:TRP:CE3	2.55	0.41
1:B:67:MET:CE	1:B:180:ALA:HB1	2.50	0.41
1:C:86:ILE:HD12	1:C:127:ILE:HG22	2.02	0.41
1:D:303:TRP:CD2	1:D:308:PRO:HD3	2.55	0.41
1:D:378:ARG:NH1	1:D:420:ASP:OD1	2.53	0.41
1:E:156:MET:HG2	1:E:210:PRO:CD	2.49	0.41
1:E:449:LEU:HD12	1:E:474:ALA:HB2	2.02	0.41
1:F:109:GLY:HA2	1:F:116:PHE:HA	2.01	0.41
1:A:329:ASN:O	1:A:330:LEU:HD23	2.20	0.41
1:B:27:ILE:O	1:B:35:CYS:HA	2.21	0.41
1:D:110:ILE:CG2	1:D:113:GLU:HB2	2.51	0.41
1:D:156:MET:O	1:D:167:THR:HA	2.20	0.41
1:E:83:TRP:N	1:E:129:LEU:O	2.51	0.41
1:A:276:GLY:O	1:A:277:LEU:HD23	2.20	0.41
1:B:69:VAL:O	1:B:72:LYS:NZ	2.38	0.41
1:A:240:TRP:HD1	1:A:278:TRP:CE3	2.39	0.41
1:A:240:TRP:CD1	1:A:316:CYS:HB3	2.56	0.41
1:A:67:MET:HG2	1:A:68:SER:N	2.36	0.41
1:B:378:ARG:NH2	1:B:420:ASP:OD2	2.53	0.41
1:C:156:MET:HG2	1:C:210:PRO:CD	2.50	0.41
1:H:378:ARG:NH2	1:H:420:ASP:OD2	2.49	0.41
1:A:27:ILE:O	1:A:35:CYS:HA	2.21	0.41
1:E:41:PRO:HA	1:E:88:LEU:HB2	2.02	0.41
1:F:426:LEU:HD23	1:F:464:VAL:HG21	2.03	0.41
1:F:86:ILE:HD13	1:F:100:TRP:HH2	1.85	0.41
1:A:421:GLU:C	1:A:422:LEU:HD23	2.41	0.41
1:C:99:LYS:HD3	1:C:111:LYS:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:LYS:HD3	1:C:245:LYS:HA	1.83	0.41
1:E:119:TYR:HB2	1:E:127:ILE:HD13	2.03	0.41
1:E:400:SER:HA	1:E:437:TRP:CZ3	2.56	0.41
1:F:240:TRP:HD1	1:F:278:TRP:CE3	2.39	0.41
1:H:27:ILE:O	1:H:35:CYS:HA	2.21	0.41
1:B:41:PRO:HD3	1:B:71:PHE:CD2	2.56	0.41
1:C:258:THR:O	1:C:299:ARG:HD2	2.21	0.41
1:D:228:VAL:HG11	1:D:341:LYS:HE3	2.03	0.41
1:E:126:ASN:ND2	1:E:127:ILE:O	2.53	0.41
1:E:392:ARG:HA	1:E:396:GLY:O	2.21	0.41
1:F:115:LEU:HB3	1:F:129:LEU:HG	2.02	0.41
1:B:300:TYR:C	1:B:301:LEU:HD12	2.40	0.41
1:D:109:GLY:HA2	1:D:116:PHE:HA	2.03	0.41
1:H:106:THR:HG21	1:H:140:LYS:HE3	2.01	0.41
1:H:29:ASN:HB2	1:H:139:TRP:CZ3	2.56	0.41
1:H:67:MET:HG2	1:H:68:SER:N	2.36	0.41
1:A:278:TRP:HZ2	1:A:334:GLN:O	2.04	0.40
1:C:252:ALA:HB1	1:C:341:LYS:O	2.22	0.40
1:C:62:SER:OG	1:C:65:GLN:HG3	2.21	0.40
1:D:376:ILE:HG13	1:D:414:LEU:HD23	2.03	0.40
1:E:292:TRP:HE1	1:E:298:PHE:HA	1.86	0.40
1:E:304:LEU:HD23	1:E:326:LYS:HD2	2.03	0.40
1:H:220:TRP:CD2	1:H:231:GLN:HB2	2.56	0.40
1:H:304:LEU:HG	1:H:326:LYS:HB2	2.02	0.40
1:A:258:THR:O	1:A:299:ARG:HD2	2.21	0.40
1:E:108:LEU:CD2	1:E:148:LEU:HD12	2.50	0.40
1:E:376:ILE:HG13	1:E:414:LEU:CD2	2.50	0.40
1:G:374:TYR:HB2	1:G:414:LEU:CD1	2.42	0.40
1:G:426:LEU:HB2	1:G:437:TRP:CZ3	2.57	0.40
1:A:303:TRP:CD2	1:A:308:PRO:HD3	2.56	0.40
1:C:311:GLU:HA	1:C:312:PRO:HD3	1.92	0.40
1:D:367:TRP:CE3	1:D:367:TRP:HA	2.56	0.40
1:F:281:LEU:HB3	1:F:317:VAL:CB	2.51	0.40
1:H:40:SER:HA	1:H:71:PHE:CE2	2.56	0.40
1:D:45:GLN:HG2	1:D:125:LYS:O	2.21	0.40
1:G:423:TRP:CE3	1:G:465:VAL:HG12	2.56	0.40
1:H:171:PRO:O	1:H:198:THR:HG23	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	439/475 (92%)	416 (95%)	22 (5%)	1 (0%)	47	79
1	B	439/475 (92%)	413 (94%)	24 (6%)	2 (0%)	29	67
1	C	435/475 (92%)	412 (95%)	22 (5%)	1 (0%)	47	79
1	D	439/475 (92%)	412 (94%)	25 (6%)	2 (0%)	29	67
1	E	440/475 (93%)	415 (94%)	23 (5%)	2 (0%)	29	67
1	F	436/475 (92%)	413 (95%)	22 (5%)	1 (0%)	47	79
1	G	439/475 (92%)	414 (94%)	23 (5%)	2 (0%)	29	67
1	H	435/475 (92%)	414 (95%)	21 (5%)	0	100	100
All	All	3502/3800 (92%)	3309 (94%)	182 (5%)	11 (0%)	41	74

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	461	GLU
1	D	461	GLU
1	G	457	ASN
1	E	105	ASP
1	G	105	ASP
1	A	105	ASP
1	B	105	ASP
1	C	105	ASP
1	D	105	ASP
1	E	457	ASN
1	F	105	ASP

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	387/418 (93%)	384 (99%)	3 (1%)	81	93
1	B	387/418 (93%)	385 (100%)	2 (0%)	88	95
1	C	385/418 (92%)	382 (99%)	3 (1%)	81	93
1	D	387/418 (93%)	384 (99%)	3 (1%)	81	93
1	E	388/418 (93%)	385 (99%)	3 (1%)	81	93
1	F	386/418 (92%)	383 (99%)	3 (1%)	81	93
1	G	387/418 (93%)	384 (99%)	3 (1%)	81	93
1	H	385/418 (92%)	382 (99%)	3 (1%)	81	93
All	All	3092/3344 (92%)	3069 (99%)	23 (1%)	84	94

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ARG
1	A	72	LYS
1	A	299	ARG
1	B	59	ARG
1	B	299	ARG
1	C	59	ARG
1	C	299	ARG
1	C	432	GLN
1	D	59	ARG
1	D	72	LYS
1	D	299	ARG
1	E	59	ARG
1	E	72	LYS
1	E	299	ARG
1	F	59	ARG
1	F	72	LYS
1	F	299	ARG
1	G	59	ARG
1	G	72	LYS
1	G	299	ARG
1	H	59	ARG
1	H	299	ARG
1	H	367	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	334	GLN
1	B	334	GLN
1	C	432	GLN
1	E	334	GLN
1	F	334	GLN
1	G	334	GLN
1	H	334	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MES	A	501	-	12,12,12	2.31	1 (8%)	14,16,16	1.59	4 (28%)
2	MES	C	501	-	12,12,12	2.29	1 (8%)	14,16,16	1.56	3 (21%)
2	MES	E	501	-	12,12,12	2.30	1 (8%)	14,16,16	1.58	4 (28%)
2	MES	H	501	-	12,12,12	2.30	1 (8%)	14,16,16	1.66	5 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MES	G	501	-	12,12,12	2.30	1 (8%)	14,16,16	1.52	4 (28%)
2	MES	B	501	-	12,12,12	2.31	1 (8%)	14,16,16	1.51	4 (28%)
2	MES	D	501	-	12,12,12	2.35	1 (8%)	14,16,16	1.48	4 (28%)
2	MES	F	501	-	12,12,12	2.32	1 (8%)	14,16,16	1.57	4 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MES	A	501	-	-	3/6/14/14	0/1/1/1
2	MES	C	501	-	-	1/6/14/14	0/1/1/1
2	MES	E	501	-	-	1/6/14/14	0/1/1/1
2	MES	H	501	-	-	2/6/14/14	0/1/1/1
2	MES	G	501	-	-	3/6/14/14	0/1/1/1
2	MES	B	501	-	-	1/6/14/14	0/1/1/1
2	MES	D	501	-	-	1/6/14/14	0/1/1/1
2	MES	F	501	-	-	1/6/14/14	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	MES	C8-S	-7.89	1.66	1.77
2	F	501	MES	C8-S	-7.78	1.66	1.77
2	A	501	MES	C8-S	-7.78	1.66	1.77
2	B	501	MES	C8-S	-7.75	1.66	1.77
2	H	501	MES	C8-S	-7.72	1.66	1.77
2	E	501	MES	C8-S	-7.70	1.66	1.77
2	G	501	MES	C8-S	-7.70	1.66	1.77
2	C	501	MES	C8-S	-7.67	1.66	1.77

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	MES	C6-C5-N4	-3.06	105.47	110.10
2	H	501	MES	C6-C5-N4	-3.01	105.54	110.10
2	F	501	MES	C6-C5-N4	-2.89	105.72	110.10
2	E	501	MES	C6-C5-N4	-2.78	105.89	110.10
2	B	501	MES	C6-C5-N4	-2.76	105.92	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	MES	C6-C5-N4	-2.74	105.94	110.10
2	G	501	MES	C6-C5-N4	-2.63	106.11	110.10
2	F	501	MES	O3S-S-C8	2.48	109.78	105.77
2	D	501	MES	C6-C5-N4	-2.46	106.37	110.10
2	E	501	MES	O3S-S-C8	2.36	109.58	105.77
2	C	501	MES	O3S-S-C8	2.31	109.50	105.77
2	H	501	MES	O1S-S-C8	2.30	109.69	106.92
2	D	501	MES	O1S-S-C8	2.30	109.69	106.92
2	H	501	MES	O3S-S-C8	2.25	109.41	105.77
2	G	501	MES	O2S-S-C8	2.25	109.63	106.92
2	A	501	MES	O3S-S-C8	2.22	109.36	105.77
2	G	501	MES	O3S-S-C8	2.22	109.35	105.77
2	B	501	MES	O3S-S-C8	2.21	109.34	105.77
2	E	501	MES	O2S-S-C8	2.19	109.55	106.92
2	H	501	MES	O2S-S-C8	2.16	109.51	106.92
2	A	501	MES	O2S-S-C8	2.15	109.51	106.92
2	A	501	MES	O1S-S-C8	2.14	109.49	106.92
2	D	501	MES	O3S-S-C8	2.14	109.22	105.77
2	C	501	MES	O2S-S-C8	2.13	109.47	106.92
2	E	501	MES	O1S-S-C8	2.11	109.46	106.92
2	B	501	MES	O2S-S-C8	2.11	109.45	106.92
2	F	501	MES	O2S-S-C8	2.10	109.45	106.92
2	D	501	MES	C5-N4-C3	2.10	113.55	108.83
2	G	501	MES	O1S-S-C8	2.07	109.41	106.92
2	B	501	MES	O1S-S-C8	2.07	109.41	106.92
2	H	501	MES	C2-C3-N4	-2.06	106.98	110.10
2	F	501	MES	C5-N4-C3	2.02	113.38	108.83

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	MES	C7-C8-S-O1S
2	G	501	MES	C7-C8-S-O2S
2	G	501	MES	C7-C8-S-O3S
2	H	501	MES	C8-C7-N4-C3
2	A	501	MES	C7-C8-S-O2S
2	G	501	MES	C7-C8-S-O1S
2	H	501	MES	C8-C7-N4-C5
2	D	501	MES	C8-C7-N4-C3
2	A	501	MES	C7-C8-S-O3S
2	C	501	MES	C8-C7-N4-C3

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Mol	Chain	Res	Type	Atoms
2	E	501	MES	C8-C7-N4-C3
2	B	501	MES	C8-C7-N4-C3
2	F	501	MES	C8-C7-N4-C3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	MES	2	0
2	G	501	MES	1	0

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	443/475 (93%)	0.14	4 (0%) 84 75	4, 11, 29, 71	0
1	B	443/475 (93%)	0.11	9 (2%) 65 51	4, 11, 32, 86	0
1	C	441/475 (92%)	0.16	7 (1%) 72 59	4, 11, 33, 97	0
1	D	443/475 (93%)	0.12	6 (1%) 75 63	4, 11, 32, 80	0
1	E	444/475 (93%)	0.16	6 (1%) 75 63	3, 11, 31, 59	0
1	F	442/475 (93%)	0.09	5 (1%) 80 69	4, 11, 30, 55	0
1	G	443/475 (93%)	0.13	7 (1%) 72 59	4, 10, 28, 58	0
1	H	441/475 (92%)	0.15	10 (2%) 60 47	5, 12, 31, 59	0
All	All	3540/3800 (93%)	0.13	54 (1%) 73 61	3, 11, 31, 97	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	456	GLU	3.3
1	C	457	ASN	3.1
1	E	480	TRP	2.9
1	B	51	GLN	2.9
1	B	480	TRP	2.8
1	G	38	ALA	2.8
1	E	133	SER	2.8
1	B	100	TRP	2.7
1	B	118	ASN	2.7
1	B	382	LYS	2.6
1	H	372	HIS	2.6
1	G	22	THR	2.6
1	C	118	ASN	2.5
1	B	123	GLN	2.5
1	D	410	ILE	2.5
1	E	112	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	121	ASN	2.4
1	E	51	GLN	2.4
1	E	413	GLN	2.4
1	B	412	SER	2.4
1	C	367	TRP	2.4
1	A	143	GLY	2.4
1	F	143	GLY	2.3
1	H	123	GLN	2.3
1	G	476	ARG	2.3
1	H	374	TYR	2.3
1	H	287	ASN	2.3
1	G	480	TRP	2.3
1	D	100	TRP	2.3
1	H	224	PRO	2.3
1	C	374	TYR	2.3
1	E	22	THR	2.2
1	H	419	ASN	2.2
1	G	393	LYS	2.2
1	B	119	TYR	2.2
1	F	385	ARG	2.2
1	C	287	ASN	2.2
1	D	458	ASN	2.2
1	A	38	ALA	2.2
1	H	36	VAL	2.2
1	H	456	GLU	2.2
1	G	444	THR	2.2
1	A	474	ALA	2.1
1	F	38	ALA	2.1
1	D	318	SER	2.1
1	D	147	ASN	2.1
1	D	121	ASN	2.1
1	C	272	SER	2.1
1	H	272	SER	2.1
1	A	481	PRO	2.1
1	H	479	GLU	2.1
1	F	64	SER	2.1
1	G	457	ASN	2.0
1	C	381	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(\AA^2)	Q<0.9
3	CA	E	502	1/1	0.81	0.17	38,38,38,38	0
3	CA	H	502	1/1	0.87	0.17	40,40,40,40	0
2	MES	G	501	12/12	0.91	0.28	16,35,56,59	0
3	CA	F	502	1/1	0.91	0.06	44,44,44,44	0
2	MES	B	501	12/12	0.92	0.16	23,39,53,57	0
2	MES	E	501	12/12	0.92	0.24	20,30,36,40	0
2	MES	C	501	12/12	0.94	0.20	15,34,61,70	0
2	MES	H	501	12/12	0.94	0.19	20,31,51,61	0
2	MES	D	501	12/12	0.94	0.15	21,36,47,47	0
2	MES	A	501	12/12	0.95	0.20	12,36,46,48	0
2	MES	F	501	12/12	0.95	0.23	16,33,43,43	0
3	CA	C	502	1/1	0.97	0.17	38,38,38,38	0
3	CA	A	502	1/1	0.97	0.11	38,38,38,38	0
3	CA	D	502	1/1	0.99	0.09	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.