



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:53 PM GMT

PDB ID : 3VB9
Title : Crystal structure of VPA0735 from *Vibrio parahaemolyticus* in monoclinic form, NorthEast Structural Genomics target VpR109
Authors : Seetharaman, J.; Neely, H.; Cunningham, K.; Ciccocanti, C.; Bjelic, S.; Acton, T.B.; Xiao, R.; Everett, J.K.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2011-12-31
Resolution : 2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

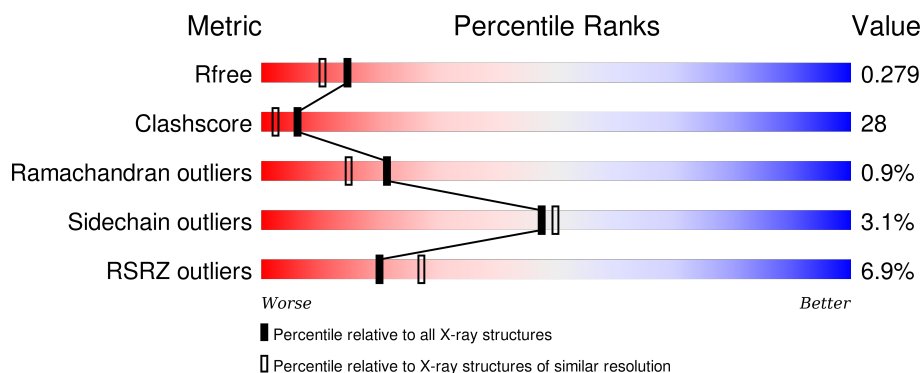
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	483	<div> <div>6%</div> <div>52%</div> <div>41%</div> <div>5%</div> </div>
1	B	483	<div> <div>10%</div> <div>51%</div> <div>42%</div> <div>• •</div> </div>
1	C	483	<div> <div>6%</div> <div>56%</div> <div>36%</div> <div>• 5%</div> </div>
1	D	483	<div> <div>4%</div> <div>61%</div> <div>33%</div> <div>• 5%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	A	502	-	-	-	X
2	MG	B	501	-	-	-	X
2	MG	B	502	-	-	-	X
2	MG	D	502	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15733 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 Uncharacterized protein VPA0735.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	Se	0	0	0
			3717	2382	623	698	14			
1	B	462	Total	C	N	O	Se	0	0	0
			3736	2393	627	702	14			
1	C	460	Total	C	N	O	Se	0	0	0
			3717	2382	623	698	14			
1	D	460	Total	C	N	O	Se	0	0	0
			3717	2382	623	698	14			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	197	Total	O	0	0
			197	197		
3	B	217	Total	O	0	0
			217	217		
3	C	190	Total	O	0	0
			190	190		
3	D	235	Total	O	0	0
			235	235		

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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.

Chain A: 6% 52% 41% 5%

Mutation	Frequency
Y311	6%
Y312	6%
K313	6%
G314	6%
T315	6%
R316	6%
W317	6%
I321	6%
S322	6%
V323	6%
S324	6%
L325	6%
D326	6%
L327	6%
D416	6%
R420	6%
K424	6%
I431	6%
Y434	6%
Y435	6%
V440	6%
G442	6%
Y443	6%
E444	6%
N451	6%
A452	6%
G453	6%
F460	6%
Y463	6%
G464	6%
P465	6%
T466	6%
A467	6%
K468	6%
M469	6%
F470	6%
D471	6%
K472	6%
S473	6%
T474	6%
L475	6%
M476	6%
G477	6%
D478	6%
I479	6%
E480	6%
L481	6%
V482	6%
LYS	6%
T222	52%
V227	52%
P228	52%
E229	52%
D231	52%
H234	52%
T235	52%
Y242	52%
W243	52%
I246	52%
H247	52%
T250	52%
Q251	52%
E252	52%
R253	52%
P254	52%
V255	52%
E257	52%
R258	52%
D259	52%
F261	52%
V262	52%
K263	52%
A264	52%
Q265	52%
G270	52%
T271	52%
G274	52%
W278	52%
E289	52%
K292	52%
V293	52%
G294	52%
R295	52%
L296	52%
R297	52%
A298	52%
Q299	52%
S300	52%
K301	52%
D302	52%
V303	52%
K305	52%
T308	52%
L146	41%
S147	41%
P151	41%
D152	41%
K153	41%
G154	41%
K155	41%
K158	41%
Y159	41%
L160	41%
I161	41%
P162	41%
P163	41%
P164	41%
G165	41%
E166	41%
K167	41%
Y168	41%
K169	41%
D170	41%
L171	41%
N172	41%
P173	41%
K174	41%
V178	41%
I179	41%
R180	41%
P181	41%
K182	41%
T183	41%
N184	41%
V185	41%
V186	41%
G189	41%
R191	41%
I192	41%
L193	41%
E194	41%
P195	41%
D196	41%
V197	41%
D198	41%
R199	41%
V200	41%
V201	41%
K202	41%
Q203	41%
V204	41%
N205	41%
P206	41%
T210	41%
D215	41%
L146	5%
S147	5%
P151	5%
D152	5%
K153	5%
G154	5%
K155	5%
K158	5%
Y159	5%
L160	5%
I161	5%
P162	5%
P163	5%
P164	5%
G165	5%
E166	5%
K167	5%
Y168	5%
K169	5%
D170	5%
L171	5%
N172	5%
P173	5%
K174	5%
V178	5%
I179	5%
R180	5%
P181	5%
K182	5%
T183	5%
N184	5%
V185	5%
V186	5%
G189	5%
R191	5%
I192	5%
L193	5%
E194	5%
P195	5%
D196	5%
V197	5%
D198	5%
R199	5%
V200	5%
V201	5%
K202	5%
Q203	5%
V204	5%
N205	5%
P206	5%
T210	5%
D215	

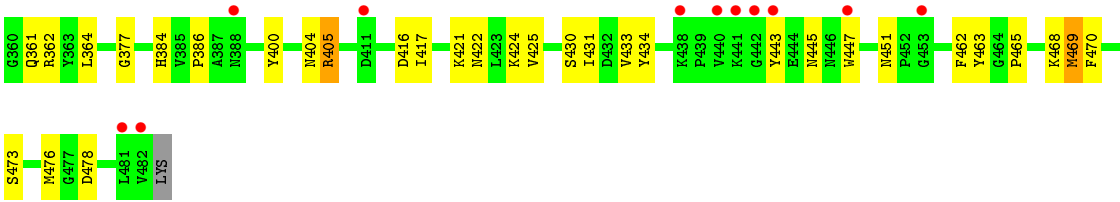
Chain B:

10% 51% 42%

MSE LVS LYS ARG ILE LEU VAL VAL THR SER MSE LEU SER ALA SER VAL PHE ALA Q22 E23 T24 V25 V26 P27 S28 R29 S37 D38 F39 P40 M45 M50 E51 M52 D53 F54 Q55 R56 L62 M63 G64 P66 A67 S68 S69 I70 M71 E72 W73 L74 M75

R78 Q87 M88 F91 R92 T93 L94 K95 Q96 K97 I101 T102 A103 M104 F105 T106 T107 P108 I109 T113 L116 I123 I124 H125 P127 E128 A129 K130 M131 M134 H139 Q140 L143 S144 D145 L146 S147 D152 K155 Y159 L160 I161 V162 P163 E166 K167

T168 K169 D170 H171 M172 P173 Y176 Y177 V178 I179 A180 P181 M184 V185 W186 Y187 I190 R191 I192 L193 E194 V197 D198 R199 V200 V201 K202 Q203 V204 V205 P206 E207 I208 T209 Q210 Q211 P212 D215 G216 V224 V227 P228 E229 D231 E234 I235 E247 Q248 I249 V250



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.27Å 106.93Å 157.18Å 90.00° 94.80° 90.00°	Depositor
Resolution (Å)	39.99 – 2.10 39.99 – 2.09	Depositor EDS
% Data completeness (in resolution range)	89.9 (39.99-2.10) 95.8 (39.99-2.09)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.63 (at 2.08Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.224 , 0.274 0.224 , 0.279	Depositor DCC
R_{free} test set	10598 reflections (9.65%)	DCC
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.831	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 61.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	3 of 237710 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	15733	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 72.02 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.3721e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.35	0/3803	0.63	3/5137 (0.1%)
1	B	0.36	0/3822	0.61	0/5160
1	C	0.34	0/3803	0.59	0/5137
1	D	0.35	0/3803	0.62	0/5137
All	All	0.35	0/15231	0.61	3/20571 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	352	MSE	N-CA-CB	-9.13	94.17	110.60
1	A	351	GLY	N-CA-C	7.81	132.62	113.10
1	A	352	MSE	N-CA-C	-5.48	96.21	111.00

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	3717	0	3643	244	0
1	B	3736	0	3664	280	0
1	C	3717	0	3643	208	0
1	D	3717	0	3643	149	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
3	A	197	0	0	12	0
3	B	217	0	0	18	0
3	C	190	0	0	11	0
3	D	235	0	0	9	0
All	All	15733	0	14593	830	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 28.

All (830) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:SER:HA	1:B:45:MSE:HE2	1.18	1.14
1:C:105:PHE:HB2	1:C:407:MSE:HE1	1.32	1.11
1:C:135:MSE:HE3	1:C:146:LEU:HD11	1.32	1.10
1:A:303:TYR:HB2	1:B:45:MSE:HE1	1.30	1.09
1:C:45:MSE:HE1	1:D:303:TYR:HB2	1.24	1.09
1:A:105:PHE:HB2	1:A:407:MSE:HE1	1.33	1.07
1:A:297:MSE:HB3	1:B:52:MSE:HE3	1.36	1.07
1:B:378:GLU:HB3	1:B:452:PRO:HD3	1.34	1.07
1:C:45:MSE:HE2	1:D:300:SER:HA	1.34	1.06
1:C:66:PRO:HA	1:C:342:PHE:CD2	1.92	1.02
1:B:392:SER:HB3	1:B:463:TYR:HB3	1.38	1.01
1:C:66:PRO:HA	1:C:342:PHE:HD2	1.26	1.01
1:D:88:MSE:HE3	1:D:210:THR:HG21	1.48	0.95
1:D:140:GLN:HE22	1:D:347:THR:H	1.17	0.92
1:B:251:GLN:HE22	1:B:274:GLY:H	1.13	0.92
1:C:330:GLU:HB3	3:C:603:HOH:O	1.68	0.91
1:A:251:GLN:HE22	1:A:274:GLY:H	1.18	0.91
1:B:415:PRO:HA	1:B:447:TRP:HZ3	1.36	0.91
1:A:70:ILE:HD11	1:A:140:GLN:HG2	1.52	0.90
1:C:397:THR:HG21	1:C:435:TYR:OH	1.72	0.90
1:C:49:LEU:HD13	1:D:306:ARG:HD2	1.50	0.90
1:D:57:ALA:HB2	1:D:269:LEU:HD21	1.53	0.89
1:D:308:THR:HG22	1:D:309:GLN:H	1.39	0.88
1:C:141:ARG:HD2	1:C:182:LYS:NZ	1.89	0.88
1:A:297:MSE:HB3	1:B:52:MSE:CE	2.05	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:VAL:HG13	1:C:198:ASP:H	1.39	0.86
1:C:140:GLN:O	1:C:140:GLN:HG2	1.75	0.86
1:C:62:LEU:HD11	1:C:297:MSE:CE	2.06	0.85
1:D:62:LEU:HD11	1:D:297:MSE:HE3	1.56	0.85
1:A:52:MSE:HE2	1:B:297:MSE:HB3	1.58	0.84
1:C:92:ASN:H	1:C:96:GLN:NE2	1.74	0.84
1:C:344:GLU:HA	1:C:405:ARG:HD2	1.60	0.84
1:A:62:LEU:HD11	1:B:52:MSE:HE2	1.60	0.83
1:A:294:GLY:HA2	1:A:297:MSE:HE2	1.58	0.83
1:A:45:MSE:HE1	1:B:303:TYR:HB2	1.61	0.83
1:A:397:THR:HG21	1:A:435:TYR:OH	1.77	0.83
1:B:134:MSE:CE	1:B:352:MSE:HE1	2.09	0.82
1:A:62:LEU:CD1	1:B:52:MSE:HE2	2.09	0.82
1:A:62:LEU:HD11	1:A:297:MSE:HE3	1.62	0.81
1:D:101:ILE:H	1:D:234:HIS:HE1	1.27	0.81
1:B:375:LEU:O	1:B:454:GLU:HG2	1.78	0.81
1:A:66:PRO:HG2	1:A:338:ARG:HG2	1.61	0.81
1:A:325:LEU:HD12	1:A:350:ARG:HH21	1.45	0.80
1:D:184:ASN:H	1:D:253:ASN:HD22	1.27	0.80
1:B:29:ARG:HB3	1:B:29:ARG:HH11	1.44	0.80
1:D:282:GLU:HG3	3:D:811:HOH:O	1.81	0.79
1:B:71:MSE:HB2	1:B:249:ILE:HD11	1.63	0.79
1:C:307:PHE:HD1	1:C:308:THR:HG23	1.46	0.79
1:D:251:GLN:HE22	1:D:274:GLY:H	1.29	0.79
1:C:263:MSE:HE1	3:C:679:HOH:O	1.83	0.79
1:A:88:MSE:HE3	1:A:210:THR:HG21	1.64	0.79
1:B:191:ARG:HH22	1:B:352:MSE:CE	1.96	0.78
1:B:390:PRO:C	1:B:465:PRO:HD2	2.04	0.78
1:B:402:GLU:HB2	1:B:454:GLU:OE2	1.84	0.78
1:C:143:LEU:HD13	1:C:181:PRO:HG3	1.66	0.78
1:A:104:ASN:HD22	1:A:104:ASN:C	1.87	0.78
1:A:184:ASN:H	1:A:253:ASN:HD22	1.32	0.77
1:B:430:SER:HB3	3:B:796:HOH:O	1.84	0.77
1:D:140:GLN:NE2	1:D:347:THR:H	1.82	0.77
1:B:397:THR:HG21	1:B:434:TYR:OH	1.85	0.76
1:B:468:LYS:HZ3	1:B:468:LYS:HB2	1.50	0.76
1:C:251:GLN:HE22	1:C:274:GLY:H	1.33	0.76
1:B:74:LEU:O	1:B:78:ARG:HG2	1.85	0.76
1:B:435:TYR:CE2	1:B:437:PRO:HD2	2.21	0.76
1:A:395:TRP:HZ2	1:A:431:ILE:HD12	1.48	0.76
1:A:300:SER:CA	1:B:45:MSE:HE2	2.08	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:MSE:SE	1:B:477:GLY:H	2.18	0.76
1:D:101:ILE:H	1:D:234:HIS:CE1	2.04	0.75
1:C:139:HIS:CD2	1:C:258:ARG:HH22	2.04	0.75
1:C:134:MSE:O	1:C:134:MSE:HE2	1.84	0.75
1:C:469:MSE:HE2	1:C:470:PHE:CD1	2.22	0.75
1:A:37:SER:HB3	1:B:454:GLU:HB3	1.68	0.75
1:C:342:PHE:HE1	1:C:347:THR:H	1.35	0.74
1:A:481:LEU:HD22	1:A:482:VAL:HG23	1.67	0.74
1:B:88:MSE:HE3	1:B:210:THR:HG21	1.69	0.74
1:A:37:SER:HB3	1:B:454:GLU:CB	2.18	0.74
1:D:294:GLY:HA2	1:D:297:MSE:HE2	1.69	0.74
1:B:215:ASP:CG	1:D:289:GLU:HG2	2.08	0.74
1:B:95:LYS:HG2	1:B:229:GLU:HG3	1.68	0.74
1:B:134:MSE:HE2	1:B:352:MSE:HE1	1.70	0.73
1:C:62:LEU:HD11	1:C:297:MSE:HE3	1.70	0.73
1:D:108:PRO:HG2	1:D:197:VAL:HG13	1.69	0.73
1:B:184:ASN:H	1:B:253:ASN:HD22	1.36	0.73
1:C:65:ILE:HB	1:C:66:PRO:HD3	1.70	0.73
1:B:390:PRO:O	1:B:465:PRO:HD2	1.87	0.73
1:B:462:PHE:O	1:B:463:TYR:HB2	1.89	0.73
1:B:415:PRO:HA	1:B:447:TRP:CZ3	2.21	0.73
1:A:45:MSE:CE	1:B:303:TYR:HB2	2.19	0.72
1:B:411:ASP:OD2	1:B:448:VAL:HG21	1.89	0.72
1:A:182:LYS:HE3	1:A:258:ARG:HH21	1.53	0.72
1:C:141:ARG:CD	1:C:182:LYS:NZ	2.53	0.72
1:A:65:ILE:HB	1:A:66:PRO:HD3	1.72	0.72
1:A:469:MSE:HE2	1:A:470:PHE:HD1	1.54	0.72
1:A:481:LEU:HD23	1:A:482:VAL:H	1.54	0.71
1:A:321:ILE:HD12	1:A:321:ILE:N	2.05	0.71
1:A:37:SER:O	1:B:454:GLU:HB3	1.90	0.71
1:C:137:ASP:OD2	1:C:182:LYS:HE2	1.90	0.71
1:D:308:THR:HG22	1:D:309:GLN:N	2.05	0.71
1:B:376:SER:HA	1:B:454:GLU:HA	1.72	0.71
1:A:481:LEU:HD23	1:A:482:VAL:N	2.05	0.71
1:B:104:ASN:HD22	1:B:104:ASN:C	1.95	0.71
1:A:45:MSE:CE	1:B:300:SER:HA	2.21	0.70
1:B:71:MSE:HB2	1:B:249:ILE:CD1	2.20	0.70
1:B:104:ASN:ND2	1:B:106:THR:H	1.89	0.70
1:A:109:TYR:HB3	1:A:111:ILE:CD1	2.21	0.70
1:B:338:ARG:CZ	3:B:601:HOH:O	2.40	0.70
1:C:199:ARG:HB2	1:C:199:ARG:HH11	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:VAL:H	1:B:253:ASN:HD21	1.39	0.70
1:B:104:ASN:HD22	1:B:106:THR:H	1.39	0.70
1:C:247:HIS:O	1:C:251:GLN:HG2	1.90	0.70
1:C:45:MSE:HE1	1:D:303:TYR:CB	2.13	0.69
1:A:124:ILE:HD13	1:A:210:THR:HG22	1.74	0.69
1:C:141:ARG:HD2	1:C:182:LYS:HZ1	1.56	0.69
1:B:161:ILE:N	1:B:161:ILE:HD12	2.07	0.69
1:B:380:THR:HG23	1:B:435:TYR:HB2	1.75	0.69
1:C:92:ASN:H	1:C:96:GLN:HE21	1.40	0.69
1:C:307:PHE:CD1	1:C:308:THR:HG23	2.28	0.69
1:C:105:PHE:HB2	1:C:407:MSE:CE	2.18	0.69
1:C:101:ILE:H	1:C:234:HIS:HE1	1.39	0.68
1:B:197:VAL:O	1:B:201:VAL:HG12	1.93	0.68
1:B:247:HIS:O	1:B:251:GLN:HG2	1.93	0.68
1:B:286:ILE:HD12	3:B:729:HOH:O	1.93	0.68
1:B:420:ARG:HB2	3:B:707:HOH:O	1.93	0.68
1:A:45:MSE:HE2	1:B:300:SER:O	1.94	0.68
1:D:75:ASN:HD21	1:D:248:GLN:HE22	1.40	0.68
1:A:185:VAL:H	1:A:253:ASN:HD21	1.43	0.67
1:A:201:VAL:O	1:A:205:VAL:HG22	1.93	0.67
1:C:62:LEU:HD11	1:C:297:MSE:HE2	1.74	0.67
1:C:469:MSE:HE2	1:C:470:PHE:HD1	1.58	0.67
1:B:65:ILE:HB	1:B:66:PRO:HD3	1.75	0.67
1:A:235:ILE:HD11	1:A:406:LEU:HD21	1.75	0.67
1:A:182:LYS:HG2	3:A:718:HOH:O	1.94	0.67
1:A:110:VAL:C	1:A:111:ILE:HD12	2.14	0.67
1:D:101:ILE:HD11	1:D:405:ARG:HB2	1.77	0.67
1:B:382:LYS:HB2	1:B:481:LEU:HD11	1.77	0.67
1:A:109:TYR:HB3	1:A:111:ILE:HD13	1.76	0.67
1:B:40:PRO:CG	1:B:45:MSE:HE3	2.25	0.66
1:B:29:ARG:HB3	1:B:29:ARG:NH1	2.09	0.66
1:A:250:ILE:HD12	1:A:263:MSE:SE	2.45	0.66
1:A:205:VAL:CG2	1:A:206:PRO:HD3	2.25	0.66
1:A:71:MSE:HE1	1:A:74:LEU:HD23	1.77	0.66
1:C:184:ASN:H	1:C:253:ASN:HD22	1.42	0.66
1:A:93:THR:OG1	1:A:96:GLN:HG3	1.95	0.66
1:B:393:ASN:H	1:B:463:TYR:HB2	1.61	0.65
1:B:440:VAL:HA	1:B:443:TYR:HE1	1.61	0.65
1:D:282:GLU:O	1:D:286:ILE:HD13	1.96	0.65
1:A:303:TYR:CB	1:B:45:MSE:HE1	2.18	0.65
1:D:185:VAL:H	1:D:253:ASN:HD21	1.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:ILE:HD12	1:C:231:ASP:H	1.61	0.65
1:C:395:TRP:HZ2	1:C:431:ILE:HD12	1.61	0.65
1:D:130:LYS:HG3	1:D:148:LEU:HD11	1.78	0.65
1:D:66:PRO:HG2	3:D:610:HOH:O	1.96	0.65
1:B:451:ASN:HB3	1:B:452:PRO:HD2	1.77	0.65
1:C:475:THR:HG22	1:C:476:MSE:N	2.12	0.64
1:B:191:ARG:HH22	1:B:352:MSE:HE2	1.61	0.64
1:B:470:PHE:CD2	1:B:472:LYS:HE3	2.33	0.64
1:B:344:GLU:HA	1:B:405:ARG:HD2	1.80	0.64
1:C:93:THR:H	1:C:96:GLN:HE21	1.44	0.64
1:A:101:ILE:H	1:A:234:HIS:HE1	1.44	0.64
1:C:349:SER:OG	1:C:352:MSE:HE3	1.98	0.64
1:A:153:LYS:HB2	1:A:155:LYS:HE2	1.80	0.64
1:B:440:VAL:HA	1:B:443:TYR:CE1	2.33	0.64
1:C:139:HIS:O	1:C:140:GLN:HB3	1.98	0.64
1:A:45:MSE:HE3	1:B:300:SER:HA	1.80	0.64
1:B:335:LEU:HA	1:B:338:ARG:HH11	1.62	0.64
1:B:382:LYS:HE3	1:B:431:ILE:HD13	1.80	0.64
1:D:465:PRO:HB2	1:D:469:MSE:HG2	1.79	0.64
1:B:391:ALA:HA	1:B:465:PRO:HD3	1.80	0.64
1:B:397:THR:O	1:B:416:ASP:HB2	1.98	0.63
1:C:93:THR:H	1:C:96:GLN:NE2	1.97	0.63
1:C:469:MSE:HE3	1:C:470:PHE:HA	1.81	0.63
1:C:101:ILE:HA	1:C:406:LEU:HD23	1.78	0.63
1:C:334:GLU:HB3	1:C:337:GLU:HB2	1.80	0.63
1:D:250:ILE:HD12	1:D:263:MSE:SE	2.48	0.63
1:D:184:ASN:H	1:D:253:ASN:ND2	1.97	0.63
1:B:250:ILE:O	1:B:273:LYS:HD3	1.99	0.63
1:B:435:TYR:CD2	1:B:437:PRO:HD2	2.34	0.63
1:B:468:LYS:HG3	1:B:469:MSE:N	2.12	0.62
1:A:469:MSE:HE2	1:A:470:PHE:CD1	2.32	0.62
1:A:104:ASN:ND2	1:A:106:THR:H	1.97	0.62
1:B:215:ASP:OD1	1:D:289:GLU:HG2	1.99	0.62
1:C:116:LEU:HD21	1:C:161:ILE:HG22	1.81	0.62
1:D:253:ASN:O	1:D:273:LYS:HE3	2.00	0.62
1:A:131:MSE:SE	1:A:190:ILE:HG21	2.49	0.62
1:A:289:GLU:HG3	1:B:29:ARG:HG3	1.82	0.62
1:B:193:LEU:HD13	1:B:463:TYR:HE1	1.65	0.62
1:A:258:ARG:NH1	3:A:601:HOH:O	2.32	0.61
1:A:39:PHE:HD1	1:B:374:TRP:HB3	1.65	0.61
1:B:29:ARG:HH11	1:B:29:ARG:CB	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ILE:CD1	1:A:140:GLN:HG2	2.28	0.61
1:B:191:ARG:NH2	1:B:352:MSE:HE2	2.15	0.61
1:A:205:VAL:HG22	1:A:206:PRO:HD3	1.83	0.61
1:C:297:MSE:HE3	1:D:52:MSE:HG3	1.81	0.61
1:A:125:ASN:HD22	1:A:158:LYS:HG2	1.66	0.61
1:C:88:MSE:HB2	1:C:224:VAL:HG22	1.83	0.61
1:D:81:PHE:HE1	1:D:230:ILE:HD11	1.66	0.61
1:B:399:VAL:HG12	1:B:408:ILE:HG21	1.83	0.60
1:C:135:MSE:HE2	1:C:188:GLY:HA2	1.83	0.60
1:D:95:LYS:HG2	1:D:229:GLU:OE2	2.01	0.60
1:C:377:GLY:O	1:C:450:THR:HG23	2.00	0.60
1:C:341:TRP:CZ3	1:C:347:THR:O	2.54	0.60
1:C:124:ILE:HD13	1:C:210:THR:HG22	1.84	0.60
1:B:172:ASN:HD22	1:B:178:VAL:HG21	1.66	0.60
1:C:242:TYR:CE2	1:C:246:ILE:HD11	2.35	0.60
1:D:183:THR:HG22	1:D:256:GLU:OE2	2.02	0.60
1:C:125:ASN:HD22	1:C:158:LYS:HG2	1.67	0.60
1:A:300:SER:HA	1:B:45:MSE:CE	2.12	0.60
1:A:270:GLY:C	1:A:271:ILE:HD12	2.22	0.60
1:D:87:GLN:C	1:D:88:MSE:HE2	2.22	0.60
1:A:71:MSE:CE	1:A:74:LEU:HD23	2.32	0.60
1:D:330:GLU:HB3	3:D:656:HOH:O	2.02	0.59
1:C:182:LYS:HG2	3:C:728:HOH:O	2.02	0.59
1:A:341:TRP:CZ3	1:A:347:THR:O	2.55	0.59
1:D:108:PRO:HB2	1:D:192:ILE:HD13	1.84	0.59
1:A:59:GLN:NE2	1:B:56:ARG:HE	2.00	0.59
1:D:101:ILE:HD13	1:D:405:ARG:O	2.02	0.59
1:B:87:GLN:C	1:B:88:MSE:HE2	2.23	0.59
1:C:436:GLY:C	1:C:450:THR:HG22	2.22	0.59
1:B:387:ALA:CB	1:B:428:ASP:HB3	2.33	0.59
1:A:182:LYS:CE	1:A:258:ARG:HH21	2.15	0.59
1:D:81:PHE:CE1	1:D:230:ILE:HD11	2.36	0.59
1:C:45:MSE:HE2	1:D:300:SER:CA	2.23	0.59
1:D:197:VAL:O	1:D:201:VAL:HG23	2.03	0.59
1:A:141:ARG:CD	1:A:182:LYS:NZ	2.66	0.59
1:D:310:PRO:HA	1:D:318:LYS:HG2	1.84	0.59
1:B:338:ARG:NE	3:B:601:HOH:O	2.36	0.59
1:A:407:MSE:O	1:A:409:ILE:HD12	2.02	0.59
1:C:101:ILE:H	1:C:234:HIS:CE1	2.21	0.59
1:B:247:HIS:HE1	1:B:275:LYS:O	1.86	0.58
1:B:418:SER:O	1:B:420:ARG:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:377:GLY:HA3	1:D:451:ASN:O	2.03	0.58
1:D:88:MSE:SE	1:D:112:GLY:HA3	2.53	0.58
1:C:185:VAL:H	1:C:253:ASN:HD21	1.51	0.58
1:C:102:THR:HA	1:C:400:TYR:CE1	2.38	0.58
1:C:197:VAL:HG13	1:C:198:ASP:N	2.15	0.58
1:A:84:GLU:H	1:A:87:GLN:HE21	1.51	0.58
1:A:235:ILE:HD11	1:A:406:LEU:CD2	2.32	0.58
1:C:141:ARG:CD	1:C:182:LYS:HZ3	2.17	0.58
1:B:377:GLY:HA3	1:B:450:THR:O	2.03	0.58
1:A:174:LYS:HB3	1:A:174:LYS:NZ	2.19	0.58
1:B:410:ASN:ND2	1:B:448:VAL:HG13	2.18	0.58
1:A:113:THR:HG23	1:A:186:VAL:O	2.04	0.58
1:D:101:ILE:HD11	1:D:405:ARG:HG3	1.85	0.58
1:B:235:ILE:HD11	1:B:406:LEU:HG	1.86	0.58
1:A:104:ASN:ND2	1:A:104:ASN:C	2.56	0.58
1:C:78:ARG:NE	1:C:85:GLU:OE2	2.31	0.58
1:C:199:ARG:HG3	1:C:203:GLN:HE22	1.68	0.58
1:A:271:ILE:N	1:A:271:ILE:HD12	2.19	0.58
1:C:141:ARG:NH1	1:C:258:ARG:CZ	2.67	0.57
1:C:124:ILE:HB	1:C:159:TYR:HB2	1.86	0.57
1:A:50:ASN:ND2	1:B:29:ARG:HH21	2.02	0.57
1:B:67:ALA:HB1	1:B:249:ILE:HD12	1.86	0.57
1:C:75:ASN:HD21	1:C:248:GLN:HE22	1.50	0.57
1:B:374:TRP:NE1	3:B:753:HOH:O	2.21	0.57
1:C:136:LEU:HD11	1:C:347:THR:OG1	2.04	0.57
1:B:50:ASN:ND2	1:B:286:ILE:HD11	2.20	0.57
1:A:246:ILE:O	1:A:250:ILE:HG12	2.04	0.57
1:D:110:VAL:HB	1:D:190:ILE:HB	1.87	0.57
1:A:172:ASN:HD22	1:A:178:VAL:HG21	1.70	0.57
1:C:325:LEU:HD12	1:C:325:LEU:H	1.70	0.57
1:A:29:ARG:HD2	1:B:54:PHE:CE2	2.40	0.57
1:B:128:GLU:HG3	1:B:155:LYS:HA	1.87	0.57
1:A:102:THR:HA	1:A:400:TYR:CE1	2.40	0.57
1:B:466:THR:HG23	1:B:470:PHE:CE1	2.38	0.56
1:C:424:LYS:NZ	1:C:424:LYS:HB2	2.20	0.56
1:B:230:ILE:HG13	1:B:231:ASP:N	2.20	0.56
1:A:58:THR:HG22	1:A:297:MSE:HE1	1.85	0.56
1:A:39:PHE:CD2	1:B:402:GLU:HG3	2.40	0.56
1:D:71:MSE:HA	1:D:71:MSE:HE3	1.87	0.56
1:D:121:PRO:HB2	1:D:213:TYR:HB3	1.86	0.56
1:A:222:ILE:HD11	3:A:777:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:PHE:CD2	1:C:227:VAL:HG21	2.41	0.56
1:D:417:ILE:CD1	1:D:433:VAL:HG13	2.36	0.56
1:B:410:ASN:CG	1:B:448:VAL:HG13	2.26	0.56
1:A:56:ARG:HD3	1:A:265:GLN:HB3	1.88	0.56
1:C:141:ARG:CD	1:C:182:LYS:HZ1	2.17	0.56
1:C:222:ILE:HD11	3:C:659:HOH:O	2.06	0.56
1:D:58:THR:HG22	1:D:297:MSE:HE1	1.87	0.56
1:D:404:ASN:O	1:D:405:ARG:HG2	2.05	0.56
1:B:101:ILE:HA	1:B:406:LEU:HD23	1.87	0.56
1:A:424:LYS:HE3	1:A:442:GLY:O	2.06	0.56
1:B:131:MSE:SE	1:B:190:ILE:HG21	2.55	0.56
1:C:135:MSE:HE3	1:C:146:LEU:CD1	2.21	0.56
1:D:315:THR:HA	1:D:478:ASP:OD2	2.05	0.56
1:B:334:GLU:HB3	1:B:337:GLU:HB2	1.88	0.56
1:C:62:LEU:CD1	1:C:297:MSE:CE	2.82	0.55
1:A:465:PRO:HB2	1:A:469:MSE:HG2	1.86	0.55
1:A:172:ASN:N	1:A:173:PRO:HD3	2.19	0.55
1:B:155:LYS:NZ	1:B:155:LYS:HB2	2.21	0.55
1:B:425:VAL:HG12	1:B:426:ASN:N	2.21	0.55
1:B:102:THR:HA	1:B:400:TYR:CE1	2.41	0.55
1:C:41:THR:OG1	1:C:43:GLU:HG2	2.06	0.55
1:A:341:TRP:CZ3	1:A:348:VAL:HG13	2.41	0.55
1:A:141:ARG:HD2	1:A:182:LYS:NZ	2.22	0.55
1:A:101:ILE:HD12	1:A:344:GLU:O	2.07	0.55
1:D:131:MSE:SE	1:D:190:ILE:HG21	2.57	0.55
1:B:104:ASN:HD21	1:B:107:THR:H	1.52	0.55
1:C:161:ILE:HD12	1:C:161:ILE:N	2.22	0.55
1:C:450:THR:HG21	3:C:663:HOH:O	2.07	0.55
1:C:282:GLU:HG3	1:C:283:GLN:N	2.22	0.55
1:A:479:ILE:N	1:A:479:ILE:HD12	2.22	0.55
1:C:111:ILE:HD13	1:C:187:TYR:OH	2.07	0.55
1:B:194:GLU:HB2	1:B:200:VAL:HG21	1.88	0.55
1:B:327:GLN:HA	1:B:334:GLU:OE1	2.07	0.55
1:A:475:THR:HG22	1:A:476:MSE:N	2.22	0.55
1:C:169:LYS:HE2	3:C:788:HOH:O	2.07	0.55
1:C:199:ARG:HB2	1:C:199:ARG:NH1	2.22	0.54
1:D:78:ARG:O	1:D:82:LYS:HA	2.07	0.54
1:A:194:GLU:HG2	3:A:768:HOH:O	2.07	0.54
1:B:398:THR:O	1:B:457:PHE:CB	2.55	0.54
1:B:235:ILE:HD11	1:B:406:LEU:CG	2.37	0.54
1:C:105:PHE:CB	1:C:407:MSE:HE1	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:440:VAL:O	1:B:441:LYS:HB3	2.08	0.54
1:D:246:ILE:O	1:D:250:ILE:HG12	2.07	0.54
1:C:56:ARG:HD3	1:C:265:GLN:HB3	1.88	0.54
1:B:91:PHE:HB2	1:B:109:TYR:HB2	1.90	0.54
1:B:93:THR:OG1	1:B:96:GLN:HG3	2.06	0.54
1:A:62:LEU:HD13	1:B:52:MSE:HE2	1.87	0.54
1:B:408:ILE:HG23	1:B:447:TRP:CH2	2.43	0.54
1:C:141:ARG:NH1	1:C:258:ARG:NH2	2.56	0.54
1:A:28:SER:HB3	1:A:33:LEU:HD21	1.90	0.54
1:A:62:LEU:HD11	1:A:297:MSE:CE	2.35	0.54
1:C:341:TRP:CH2	1:C:347:THR:O	2.60	0.54
1:A:295:ARG:NE	3:A:635:HOH:O	2.41	0.54
1:D:58:THR:HG22	1:D:297:MSE:CE	2.37	0.54
1:A:78:ARG:NH2	1:A:118:LYS:HE2	2.23	0.54
1:D:30:VAL:HG11	1:D:51:GLU:HG2	1.88	0.54
1:C:135:MSE:CE	1:C:188:GLY:HA2	2.37	0.54
1:B:102:THR:HG21	1:B:456:TRP:CH2	2.43	0.54
1:B:97:LYS:HE2	1:B:109:TYR:CD2	2.43	0.54
1:B:408:ILE:HG12	1:B:447:TRP:HZ2	1.72	0.53
1:D:308:THR:CG2	1:D:309:GLN:H	2.18	0.53
1:B:185:VAL:H	1:B:253:ASN:ND2	2.06	0.53
1:A:128:GLU:HG3	1:A:155:LYS:HA	1.91	0.53
1:B:172:ASN:ND2	1:B:178:VAL:HG21	2.24	0.53
1:D:247:HIS:HE1	1:D:275:LYS:O	1.91	0.53
1:A:104:ASN:HD22	1:A:106:THR:H	1.55	0.53
1:B:78:ARG:HD2	3:B:728:HOH:O	2.08	0.53
1:C:378:GLU:HG2	1:C:379:HIS:CD2	2.44	0.53
1:A:166:GLU:H	1:A:166:GLU:CD	2.12	0.53
1:B:381:TYR:HD2	1:B:449:GLN:HE22	1.56	0.53
1:A:469:MSE:HG3	1:A:470:PHE:N	2.23	0.53
1:D:135:MSE:HE2	1:D:188:GLY:CA	2.38	0.53
1:D:425:VAL:HA	1:D:431:ILE:CD1	2.38	0.53
1:C:135:MSE:HA	1:C:135:MSE:HE2	1.91	0.53
1:A:45:MSE:HE2	1:B:300:SER:HA	1.90	0.53
1:A:161:ILE:HD12	1:A:161:ILE:N	2.24	0.53
1:B:191:ARG:HH22	1:B:352:MSE:HE1	1.72	0.53
1:B:382:LYS:HG3	1:B:431:ILE:HG23	1.89	0.53
1:A:242:TYR:CE1	1:A:246:ILE:HD11	2.43	0.53
1:A:315:THR:HA	1:A:478:ASP:OD2	2.09	0.53
1:B:468:LYS:HE2	3:B:677:HOH:O	2.08	0.53
1:D:131:MSE:SE	1:D:190:ILE:CG2	3.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:361:GLN:HG2	1:C:463:TYR:CZ	2.44	0.53
1:D:101:ILE:CD1	1:D:405:ARG:HB2	2.39	0.53
1:B:104:ASN:ND2	1:B:104:ASN:C	2.60	0.53
1:B:285:LYS:HB2	3:B:729:HOH:O	2.10	0.52
1:B:102:THR:HG21	1:B:456:TRP:HH2	1.74	0.52
1:D:101:ILE:HD12	1:D:344:GLU:O	2.10	0.52
1:A:334:GLU:O	1:A:338:ARG:HB2	2.08	0.52
1:B:101:ILE:H	1:B:234:HIS:CE1	2.28	0.52
1:A:378:GLU:HG2	1:A:379:HIS:ND1	2.24	0.52
1:A:137:ASP:OD2	1:A:182:LYS:HE2	2.09	0.52
1:D:417:ILE:HD13	1:D:433:VAL:HG13	1.92	0.52
1:A:87:GLN:C	1:A:88:MSE:HE2	2.29	0.52
1:C:331:ASN:HB3	1:D:255:VAL:HG21	1.90	0.52
1:D:172:ASN:N	1:D:173:PRO:HD3	2.25	0.52
1:A:39:PHE:CD1	1:B:374:TRP:HB3	2.45	0.52
1:C:347:THR:HG23	1:C:352:MSE:HE1	1.91	0.52
1:B:40:PRO:HG2	1:B:45:MSE:HE3	1.91	0.52
1:D:114:TRP:HE1	1:D:116:LEU:HD23	1.74	0.52
1:A:72:GLU:OE1	1:A:72:GLU:HA	2.09	0.52
1:C:475:THR:CG2	1:C:476:MSE:N	2.72	0.52
1:C:182:LYS:HE3	1:C:258:ARG:HH21	1.75	0.52
1:D:199:ARG:O	1:D:203:GLN:HG3	2.10	0.52
1:B:29:ARG:HD2	3:B:762:HOH:O	2.10	0.51
1:A:101:ILE:HD13	1:A:405:ARG:O	2.11	0.51
1:B:187:TYR:C	1:B:187:TYR:CD1	2.83	0.51
1:A:66:PRO:CG	1:A:338:ARG:HG2	2.36	0.51
1:D:108:PRO:CG	1:D:197:VAL:HG13	2.39	0.51
1:C:131:MSE:HE2	1:C:190:ILE:HG22	1.91	0.51
1:D:101:ILE:HG23	1:D:345:ALA:HA	1.92	0.51
1:A:101:ILE:H	1:A:234:HIS:CE1	2.26	0.51
1:A:111:ILE:N	1:A:111:ILE:HD12	2.25	0.51
1:A:468:LYS:HD3	3:A:693:HOH:O	2.09	0.51
1:B:451:ASN:O	1:B:453:GLY:N	2.42	0.51
1:B:387:ALA:HB1	1:B:428:ASP:HB3	1.93	0.51
1:D:361:GLN:HG2	1:D:463:TYR:CZ	2.45	0.51
1:B:129:ALA:HB3	1:B:131:MSE:HE2	1.93	0.51
1:B:341:TRP:HE1	1:B:348:VAL:CG1	2.24	0.51
1:B:321:ILE:N	1:B:321:ILE:HD12	2.25	0.51
1:A:441:LYS:HG3	1:A:441:LYS:O	2.11	0.51
1:D:57:ALA:HB2	1:D:269:LEU:CD2	2.35	0.51
1:C:295:ARG:HG3	1:C:295:ARG:HH11	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:LEU:HD21	1:C:161:ILE:CG2	2.39	0.51
1:B:101:ILE:H	1:B:234:HIS:HE1	1.59	0.51
1:B:335:LEU:HD12	1:B:338:ARG:NH1	2.26	0.51
1:B:172:ASN:N	1:B:173:PRO:HD3	2.25	0.51
1:D:30:VAL:HG12	1:D:30:VAL:O	2.09	0.51
1:D:101:ILE:HD11	1:D:405:ARG:CG	2.40	0.51
1:C:126:LEU:HD21	1:C:190:ILE:CD1	2.40	0.51
1:B:147:SER:HA	1:B:152:ASP:OD1	2.11	0.51
1:C:140:GLN:CD	1:C:342:PHE:CD1	2.85	0.50
1:A:140:GLN:NE2	1:A:346:ILE:HD12	2.26	0.50
1:A:305:LYS:HE3	3:A:733:HOH:O	2.11	0.50
1:A:313:LYS:HZ2	1:A:314:GLY:CA	2.24	0.50
1:B:285:LYS:O	1:B:289:GLU:HG3	2.09	0.50
1:B:467:GLU:HA	1:B:472:LYS:HD2	1.93	0.50
1:B:40:PRO:HG3	1:B:45:MSE:HE3	1.92	0.50
1:C:45:MSE:CE	1:D:303:TYR:HB2	2.17	0.50
1:D:404:ASN:C	1:D:405:ARG:HG2	2.31	0.50
1:B:335:LEU:HA	1:B:338:ARG:NH1	2.26	0.50
1:C:230:ILE:HD12	1:C:231:ASP:N	2.25	0.50
1:A:302:ASP:O	1:A:305:LYS:HG3	2.11	0.50
1:D:240:LEU:HG	1:D:288:LEU:HD21	1.92	0.50
1:C:390:PRO:HB2	1:C:469:MSE:HB3	1.92	0.50
1:A:29:ARG:NH1	1:A:29:ARG:HG3	2.26	0.50
1:B:408:ILE:HG12	1:B:447:TRP:CZ2	2.47	0.50
1:A:185:VAL:H	1:A:253:ASN:ND2	2.09	0.50
1:D:425:VAL:HG22	1:D:431:ILE:HD11	1.93	0.50
1:B:464:GLY:N	3:B:783:HOH:O	2.40	0.50
1:C:146:LEU:O	1:C:147:SER:HB3	2.12	0.50
1:C:73:TRP:CZ3	1:C:346:ILE:HD13	2.46	0.50
1:C:88:MSE:HE3	1:C:210:THR:HG21	1.93	0.50
1:A:341:TRP:HZ3	1:A:348:VAL:HG13	1.77	0.50
1:D:192:ILE:N	1:D:192:ILE:HD12	2.27	0.50
1:B:467:GLU:HG3	3:B:724:HOH:O	2.11	0.50
1:B:230:ILE:HD12	1:B:231:ASP:H	1.75	0.50
1:A:28:SER:HB3	1:A:33:LEU:CD2	2.41	0.50
1:A:91:PHE:CD2	1:A:227:VAL:HG21	2.47	0.49
1:C:182:LYS:HG3	1:C:183:THR:HG23	1.94	0.49
1:A:139:HIS:CD2	1:A:258:ARG:HH22	2.30	0.49
1:D:230:ILE:HD13	1:D:230:ILE:H	1.76	0.49
1:D:123:ILE:HD13	1:D:160:LEU:HD13	1.94	0.49
1:C:40:PRO:CG	1:C:45:MSE:HE3	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ARG:HH11	1:A:29:ARG:HG3	1.77	0.49
1:A:313:LYS:NZ	3:A:764:HOH:O	2.45	0.49
1:C:71:MSE:HE1	1:C:74:LEU:HD23	1.95	0.49
1:A:235:ILE:HD11	1:A:406:LEU:CG	2.42	0.49
1:C:91:PHE:HB2	1:C:109:TYR:HB2	1.94	0.49
1:B:356:ILE:N	1:B:356:ILE:HD12	2.27	0.49
1:D:302:ASP:O	1:D:305:LYS:HG3	2.13	0.49
1:A:408:ILE:HD13	1:A:409:ILE:N	2.28	0.49
1:C:166:GLU:OE1	1:C:166:GLU:HA	2.11	0.49
1:A:37:SER:O	1:A:38:ASP:HB2	2.13	0.49
1:D:123:ILE:HG22	1:D:124:ILE:N	2.28	0.49
1:D:123:ILE:CD1	1:D:160:LEU:HD13	2.42	0.49
1:B:215:ASP:HB2	1:C:28:SER:C	2.33	0.49
1:A:133:GLY:HA3	1:A:190:ILE:HD13	1.95	0.49
1:A:37:SER:HB3	1:B:454:GLU:HB2	1.91	0.49
1:C:141:ARG:HD2	1:C:182:LYS:CE	2.42	0.49
1:D:430:SER:O	1:D:431:ILE:HD13	2.13	0.49
1:D:102:THR:HA	1:D:400:TYR:CE1	2.47	0.49
1:C:141:ARG:CZ	1:C:182:LYS:HZ1	2.25	0.49
1:A:243:TRP:CZ3	1:A:246:ILE:HD12	2.48	0.49
1:B:230:ILE:CG1	1:B:231:ASP:N	2.76	0.49
1:B:398:THR:HA	1:B:416:ASP:HB3	1.94	0.48
1:B:476:MSE:CG	1:B:477:GLY:N	2.76	0.48
1:A:197:VAL:HG23	1:A:198:ASP:N	2.28	0.48
1:B:194:GLU:CB	1:B:200:VAL:HG21	2.43	0.48
1:A:363:TYR:N	1:A:363:TYR:CD1	2.81	0.48
1:D:196:ASP:HB2	3:D:807:HOH:O	2.13	0.48
1:A:141:ARG:NH1	1:A:258:ARG:CZ	2.77	0.48
1:B:69:SER:OG	1:B:346:ILE:HD13	2.12	0.48
1:A:303:TYR:HB2	1:B:45:MSE:CE	2.23	0.48
1:A:380:THR:O	1:A:482:VAL:N	2.46	0.48
1:C:199:ARG:HG3	1:C:203:GLN:NE2	2.27	0.48
1:C:111:ILE:HG12	1:C:189:GLY:HA2	1.96	0.48
1:B:341:TRP:HE1	1:B:348:VAL:HG13	1.77	0.48
1:A:444:GLU:H	1:A:444:GLU:CD	2.17	0.48
1:A:341:TRP:HZ3	1:A:347:THR:O	1.97	0.48
1:B:134:MSE:HE1	1:B:352:MSE:HE1	1.92	0.48
1:C:322:SER:HB2	3:C:660:HOH:O	2.13	0.48
1:B:63:TRP:HA	1:B:335:LEU:HD11	1.96	0.48
1:A:381:TYR:HB3	1:A:479:ILE:CG2	2.44	0.48
1:A:52:MSE:O	1:A:56:ARG:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:GLU:HG2	3:A:790:HOH:O	2.13	0.48
1:B:251:GLN:O	1:B:273:LYS:HE3	2.13	0.48
1:C:405:ARG:NH1	3:C:680:HOH:O	2.46	0.48
1:A:141:ARG:CD	1:A:182:LYS:HZ3	2.26	0.48
1:C:255:VAL:HG21	1:D:331:ASN:HB3	1.95	0.48
1:D:205:VAL:HB	1:D:206:PRO:HD3	1.95	0.48
1:C:182:LYS:CE	1:C:258:ARG:HH21	2.27	0.48
1:D:266:LEU:HD23	1:D:269:LEU:HD22	1.94	0.48
1:B:335:LEU:CD1	1:B:338:ARG:HH12	2.27	0.48
1:A:141:ARG:CZ	1:A:182:LYS:HZ1	2.27	0.48
1:B:139:HIS:HD2	3:B:633:HOH:O	1.96	0.48
1:D:100:ILE:HB	1:D:103:ALA:HB2	1.95	0.48
1:C:121:PRO:HB2	1:C:213:TYR:O	2.14	0.47
1:C:321:ILE:HD12	1:C:341:TRP:CZ2	2.49	0.47
1:D:143:LEU:HD11	1:D:181:PRO:HB3	1.96	0.47
1:C:235:ILE:HD11	1:C:406:LEU:HG	1.95	0.47
1:B:390:PRO:HB2	1:B:468:LYS:HB3	1.96	0.47
1:D:87:GLN:NE2	1:D:225:ALA:HB2	2.29	0.47
1:D:101:ILE:HD11	1:D:405:ARG:CB	2.44	0.47
1:A:115:ASN:OD1	1:A:117:GLU:HB3	2.14	0.47
1:C:143:LEU:CD1	1:C:181:PRO:HG3	2.43	0.47
1:D:27:PRO:HB3	3:D:645:HOH:O	2.15	0.47
1:C:70:ILE:HD13	1:C:346:ILE:HD11	1.97	0.47
1:A:289:GLU:HG3	1:B:29:ARG:HD2	1.96	0.47
1:D:247:HIS:O	1:D:251:GLN:HG2	2.14	0.47
1:A:395:TRP:CZ2	1:A:431:ILE:HD12	2.39	0.47
1:B:140:GLN:NE2	1:B:346:ILE:HD12	2.30	0.47
1:D:226:GLN:HG2	3:D:718:HOH:O	2.14	0.47
1:A:51:GLU:O	1:A:55:GLN:HG3	2.14	0.47
1:A:192:ILE:N	1:A:192:ILE:HD12	2.29	0.47
1:B:37:SER:O	1:B:38:ASP:HB2	2.14	0.47
1:A:420:ARG:HH11	1:A:420:ARG:HG2	1.80	0.47
1:C:100:ILE:HB	1:C:103:ALA:HB2	1.96	0.47
1:B:392:SER:HB3	1:B:463:TYR:CB	2.27	0.47
1:B:72:GLU:OE1	1:B:72:GLU:HA	2.15	0.47
1:B:435:TYR:O	1:B:448:VAL:HA	2.14	0.47
1:B:461:ARG:CG	1:B:461:ARG:HH11	2.28	0.47
1:D:62:LEU:CD1	1:D:297:MSE:HE3	2.35	0.47
1:A:78:ARG:O	1:A:82:LYS:HA	2.14	0.47
1:B:215:ASP:OD2	1:D:289:GLU:HG2	2.14	0.46
1:A:182:LYS:HD2	1:A:256:GLU:OE1	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:ASN:HD21	1:D:248:GLN:NE2	2.11	0.46
1:C:197:VAL:O	1:C:201:VAL:HG23	2.15	0.46
1:A:460:PHE:CD2	1:A:476:MSE:HE1	2.51	0.46
1:B:310:PRO:HA	1:B:318:LYS:HG2	1.96	0.46
1:C:66:PRO:CA	1:C:342:PHE:CD2	2.83	0.46
1:A:184:ASN:H	1:A:253:ASN:ND2	2.07	0.46
1:D:50:ASN:ND2	1:D:286:ILE:HD11	2.30	0.46
1:B:184:ASN:H	1:B:253:ASN:ND2	2.07	0.46
1:B:108:PRO:CG	1:B:197:VAL:HG13	2.45	0.46
1:B:434:TYR:HB3	1:B:447:TRP:HD1	1.81	0.46
1:A:469:MSE:HE3	1:A:470:PHE:HA	1.97	0.46
1:B:22:GLN:HE21	1:B:22:GLN:HB2	1.59	0.46
1:D:124:ILE:CD1	1:D:210:THR:HG22	2.45	0.46
1:B:201:VAL:HG23	1:B:205:VAL:HG21	1.96	0.46
1:C:111:ILE:CG2	1:C:112:GLY:N	2.79	0.46
1:A:135:MSE:HE2	1:A:161:ILE:HG12	1.97	0.46
1:D:424:LYS:HD3	1:D:443:TYR:CE1	2.51	0.46
1:C:363:TYR:N	1:C:363:TYR:CD1	2.83	0.46
1:C:67:ALA:HA	1:C:138:VAL:O	2.15	0.46
1:B:435:TYR:N	1:B:449:GLN:HG3	2.30	0.46
1:B:387:ALA:HB2	1:B:428:ASP:HB3	1.96	0.46
1:B:70:ILE:CD1	1:B:346:ILE:HD11	2.46	0.46
1:D:72:GLU:OE1	1:D:72:GLU:HA	2.15	0.46
1:B:377:GLY:HA2	1:B:449:GLN:HB3	1.96	0.46
1:B:457:PHE:HZ	1:B:478:ASP:CG	2.19	0.46
1:A:235:ILE:HD13	1:A:404:ASN:O	2.16	0.46
1:A:365:VAL:HG22	1:A:366:THR:N	2.30	0.46
1:B:355:THR:H	1:B:356:ILE:HD12	1.81	0.46
1:A:335:LEU:HD21	3:A:657:HOH:O	2.16	0.46
1:B:251:GLN:HE22	1:B:274:GLY:N	1.96	0.46
1:A:366:THR:HG21	1:A:479:ILE:CD1	2.46	0.46
1:A:312:TRP:CZ3	1:A:476:MSE:HB3	2.51	0.46
1:D:322:SER:HB2	3:D:626:HOH:O	2.14	0.46
1:B:75:ASN:HD21	1:B:248:GLN:HE22	1.63	0.46
1:B:468:LYS:HZ3	1:B:468:LYS:CB	2.24	0.45
1:A:84:GLU:H	1:A:87:GLN:NE2	2.13	0.45
1:B:229:GLU:HG2	3:B:770:HOH:O	2.15	0.45
1:A:182:LYS:CD	1:A:256:GLU:OE1	2.64	0.45
1:C:235:ILE:HD11	1:C:406:LEU:CG	2.46	0.45
1:C:417:ILE:HG23	1:C:423:LEU:HD21	1.99	0.45
1:B:384:HIS:O	1:B:386:PRO:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:PRO:C	1:B:465:PRO:CD	2.81	0.45
1:A:183:THR:CG2	1:A:256:GLU:OE2	2.64	0.45
1:A:101:ILE:HD13	1:A:102:THR:N	2.32	0.45
1:C:279:PRO:HB2	1:C:284:LYS:CG	2.46	0.45
1:A:199:ARG:O	1:A:203:GLN:HG3	2.15	0.45
1:C:128:GLU:O	1:C:129:ALA:HB2	2.17	0.45
1:B:434:TYR:HB3	1:B:449:GLN:HE21	1.82	0.45
1:D:71:MSE:HE1	1:D:74:LEU:HD23	1.98	0.45
1:C:342:PHE:CZ	1:C:346:ILE:HG13	2.51	0.45
1:A:91:PHE:HB2	1:A:109:TYR:HB2	1.99	0.45
1:D:201:VAL:HG13	1:D:205:VAL:HG21	1.98	0.45
1:A:171:LEU:O	1:A:180:ARG:NH2	2.49	0.45
1:D:149:LEU:HD21	1:D:359:PHE:HB3	1.98	0.45
1:D:468:LYS:HG2	1:D:473:SER:OG	2.16	0.45
1:A:261:PHE:O	1:A:265:GLN:HG3	2.17	0.45
1:C:308:THR:HG21	1:C:322:SER:OG	2.16	0.45
1:C:48:MSE:HA	1:C:48:MSE:HE2	1.99	0.45
1:B:352:MSE:HG2	1:B:363:TYR:CE1	2.51	0.45
1:B:108:PRO:HG2	1:B:197:VAL:HG13	1.98	0.45
1:A:194:GLU:CB	1:A:200:VAL:HG21	2.47	0.45
1:C:279:PRO:HB2	1:C:284:LYS:HG3	1.98	0.45
1:B:198:ASP:OD1	1:B:202:LYS:HE3	2.16	0.45
1:A:136:LEU:HD11	1:A:347:THR:HA	1.99	0.45
1:A:142:VAL:HG21	1:A:325:LEU:HD22	1.99	0.45
1:B:104:ASN:HB2	3:B:808:HOH:O	2.16	0.45
1:B:470:PHE:O	1:B:471:ASP:HB2	2.17	0.45
1:C:131:MSE:SE	1:C:190:ILE:HG21	2.67	0.45
1:A:164:PRO:HD2	3:A:627:HOH:O	2.16	0.45
1:C:141:ARG:NE	1:C:182:LYS:HZ1	2.15	0.45
1:C:115:ASN:OD1	1:C:117:GLU:HB3	2.17	0.45
1:B:361:GLN:HA	1:B:461:ARG:O	2.17	0.44
1:D:416:ASP:O	1:D:417:ILE:HG13	2.17	0.44
1:B:261:PHE:O	1:B:265:GLN:HG3	2.16	0.44
1:A:308:THR:HG21	1:A:322:SER:OG	2.16	0.44
1:D:184:ASN:N	1:D:253:ASN:HD22	2.04	0.44
1:C:305:LYS:HG2	1:C:307:PHE:CE1	2.53	0.44
1:A:255:VAL:HG22	1:A:263:MSE:HE3	1.99	0.44
1:D:421:LYS:HE2	1:D:445:ASN:HB3	1.99	0.44
1:A:39:PHE:CD1	1:B:454:GLU:HG3	2.53	0.44
1:B:457:PHE:HZ	1:B:478:ASP:OD2	2.00	0.44
1:A:111:ILE:HG13	1:A:189:GLY:HA2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:SER:O	1:B:428:ASP:CB	2.66	0.44
1:A:361:GLN:HG2	1:A:463:TYR:CE1	2.53	0.44
1:B:390:PRO:HG2	1:B:473:SER:HB3	1.99	0.44
1:A:194:GLU:HB2	1:A:200:VAL:HG21	1.99	0.44
1:A:361:GLN:HG2	1:A:463:TYR:CZ	2.51	0.44
1:B:126:LEU:HA	1:B:127:PRO:HD3	1.86	0.44
1:C:393:ASN:O	1:C:394:PHE:HB3	2.16	0.44
1:B:475:THR:HG22	1:B:476:MSE:N	2.32	0.44
1:C:151:PRO:HG2	1:C:159:TYR:OH	2.18	0.44
1:B:159:TYR:HD2	1:B:179:ILE:HD11	1.81	0.44
1:A:292:LYS:HD3	1:B:26:VAL:HG12	2.00	0.44
1:B:362:ARG:HD2	1:B:362:ARG:HA	1.85	0.44
1:C:183:THR:CG2	1:C:256:GLU:OE2	2.66	0.44
1:C:136:LEU:HD11	1:C:347:THR:HA	1.99	0.44
1:C:347:THR:HG23	1:C:352:MSE:SE	2.67	0.44
1:A:481:LEU:CD2	1:A:482:VAL:HG23	2.41	0.44
1:A:366:THR:HG21	1:A:479:ILE:HD13	2.00	0.44
1:C:277:PHE:CE1	1:C:279:PRO:HG3	2.52	0.44
1:D:319:ASP:HA	1:D:364:LEU:HD23	2.00	0.44
1:B:280:THR:OG1	1:B:283:GLN:HG3	2.17	0.44
1:B:457:PHE:CZ	1:B:478:ASP:OD2	2.71	0.44
1:A:346:ILE:C	1:A:347:THR:HG23	2.38	0.44
1:B:215:ASP:HB2	1:C:28:SER:HA	1.99	0.44
1:B:341:TRP:NE1	1:B:348:VAL:CG1	2.80	0.44
1:A:163:PRO:HA	1:A:164:PRO:HD3	1.86	0.44
1:D:73:TRP:CZ3	1:D:346:ILE:HD13	2.53	0.44
1:D:27:PRO:HB2	3:D:835:HOH:O	2.18	0.44
1:B:378:GLU:CB	1:B:452:PRO:HD3	2.24	0.44
1:B:399:VAL:HA	1:B:457:PHE:HB3	2.00	0.44
1:B:476:MSE:HG3	1:B:477:GLY:N	2.33	0.44
1:C:389:VAL:HA	1:C:390:PRO:HD3	1.87	0.44
1:A:111:ILE:CG2	1:A:112:GLY:N	2.81	0.44
1:C:71:MSE:CE	1:C:74:LEU:HD23	2.47	0.44
1:C:213:TYR:CD1	1:C:213:TYR:C	2.91	0.44
1:C:464:GLY:N	1:C:465:PRO:CD	2.81	0.44
1:C:235:ILE:HD11	1:C:406:LEU:HD21	1.99	0.43
1:C:312:TRP:CG	1:C:475:THR:HG23	2.53	0.43
1:C:141:ARG:HH12	1:C:258:ARG:CZ	2.31	0.43
1:B:230:ILE:CD1	1:B:231:ASP:H	2.30	0.43
1:B:425:VAL:HG12	1:B:426:ASN:H	1.82	0.43
1:C:341:TRP:HZ3	1:C:348:VAL:HB	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ASN:HD21	1:B:286:ILE:HD11	1.83	0.43
1:C:87:GLN:C	1:C:88:MSE:HE2	2.38	0.43
1:C:436:GLY:CA	1:C:450:THR:HG22	2.48	0.43
1:D:211:GLN:CD	1:D:221:LYS:HD3	2.39	0.43
1:A:25:VAL:HG22	1:A:34:LYS:HG2	2.00	0.43
1:B:375:LEU:HD13	1:B:457:PHE:CE1	2.53	0.43
1:C:182:LYS:HD2	1:C:256:GLU:OE1	2.19	0.43
1:A:342:PHE:HZ	1:A:348:VAL:CG2	2.31	0.43
1:C:380:THR:HA	1:C:435:TYR:O	2.18	0.43
1:C:255:VAL:HG22	1:C:263:MSE:HE3	2.00	0.43
1:C:203:GLN:O	1:C:207:ASN:ND2	2.51	0.43
1:A:235:ILE:HD11	1:A:406:LEU:HG	1.99	0.43
1:D:362:ARG:HA	1:D:362:ARG:HD2	1.76	0.43
1:B:379:HIS:HB3	1:B:480:GLU:OE2	2.19	0.43
1:A:321:ILE:HG13	1:A:341:TRP:CE2	2.53	0.43
1:A:380:THR:HA	1:A:435:TYR:O	2.18	0.43
1:D:425:VAL:HA	1:D:431:ILE:HD13	1.99	0.43
1:D:91:PHE:HB2	1:D:109:TYR:HB2	2.00	0.43
1:A:408:ILE:HD11	1:A:451:ASN:OD1	2.18	0.43
1:A:251:GLN:HE22	1:A:274:GLY:N	2.00	0.43
1:B:95:LYS:CG	1:B:229:GLU:HG3	2.44	0.43
1:B:104:ASN:ND2	1:B:107:THR:H	2.15	0.43
1:A:312:TRP:CG	1:A:475:THR:HG23	2.54	0.43
1:B:410:ASN:CB	1:B:448:VAL:HG13	2.49	0.43
1:D:469:MSE:HG3	1:D:470:PHE:N	2.33	0.43
1:B:162:VAL:HA	1:B:163:PRO:HD3	1.86	0.43
1:C:40:PRO:HG2	1:C:45:MSE:HE3	2.01	0.43
1:B:408:ILE:HD12	1:B:409:ILE:N	2.34	0.43
1:B:161:ILE:N	1:B:161:ILE:CD1	2.76	0.43
1:B:382:LYS:HE3	1:B:431:ILE:HG21	2.01	0.43
1:D:97:LYS:HE2	1:D:109:TYR:CD2	2.54	0.43
1:A:390:PRO:HD3	1:A:474:TRP:CD2	2.54	0.43
1:C:384:HIS:O	1:C:386:PRO:HD3	2.18	0.43
1:D:194:GLU:HA	1:D:195:PRO:HD3	1.83	0.43
1:C:481:LEU:HD13	1:C:481:LEU:C	2.39	0.43
1:B:123:ILE:HD13	1:B:176:TYR:HE2	1.83	0.43
1:B:143:LEU:CD1	1:B:181:PRO:HB3	2.49	0.43
1:C:147:SER:HA	1:C:152:ASP:OD2	2.19	0.43
1:B:193:LEU:HD13	1:B:463:TYR:CE1	2.51	0.43
1:B:124:ILE:CD1	1:B:210:THR:HG22	2.49	0.43
1:A:130:LYS:HD2	1:A:194:GLU:CD	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:GLU:HG3	3:C:686:HOH:O	2.18	0.43
1:C:73:TRP:HZ3	1:C:346:ILE:HD13	1.83	0.43
1:A:475:THR:CG2	1:A:476:MSE:N	2.81	0.43
1:C:421:LYS:HG2	1:C:422:ASN:N	2.34	0.43
1:D:148:LEU:O	1:D:153:LYS:HA	2.19	0.42
1:C:439:PRO:HG3	1:C:447:TRP:CZ3	2.54	0.42
1:D:174:LYS:HG3	3:D:780:HOH:O	2.19	0.42
1:B:467:GLU:HG2	1:B:472:LYS:HD2	2.00	0.42
1:C:172:ASN:N	1:C:173:PRO:HD3	2.34	0.42
1:B:461:ARG:CG	1:B:461:ARG:NH1	2.83	0.42
1:A:247:HIS:O	1:A:251:GLN:HG2	2.19	0.42
1:B:205:VAL:HB	1:B:206:PRO:HD3	2.00	0.42
1:B:382:LYS:HE3	1:B:431:ILE:CG2	2.49	0.42
1:C:91:PHE:CE2	1:C:227:VAL:HG21	2.54	0.42
1:A:195:PRO:HD2	3:A:741:HOH:O	2.19	0.42
1:C:56:ARG:HB3	1:C:265:GLN:HB3	2.01	0.42
1:D:135:MSE:HE2	1:D:188:GLY:HA3	2.00	0.42
1:A:391:ALA:HA	1:A:464:GLY:O	2.19	0.42
1:A:342:PHE:CZ	1:A:348:VAL:HG22	2.55	0.42
1:C:57:ALA:HB2	1:C:269:LEU:CD1	2.50	0.42
1:B:211:GLN:HA	1:B:212:PRO:HD3	1.93	0.42
1:C:475:THR:CG2	1:C:476:MSE:H	2.33	0.42
1:D:462:PHE:CE2	1:D:469:MSE:HE3	2.54	0.42
1:D:230:ILE:HD13	1:D:230:ILE:N	2.34	0.42
1:D:166:GLU:OE2	1:D:169:LYS:HD2	2.19	0.42
1:C:211:GLN:HA	1:C:212:PRO:HD3	1.83	0.42
1:A:45:MSE:HE1	1:B:304:THR:N	2.34	0.42
1:B:468:LYS:C	1:B:468:LYS:HZ2	2.22	0.42
1:B:70:ILE:HD13	1:B:346:ILE:HD11	2.00	0.42
1:A:143:LEU:HD11	1:A:181:PRO:HB3	2.02	0.42
1:A:48:MSE:HA	1:A:48:MSE:HE2	2.02	0.42
1:A:205:VAL:HG23	1:A:206:PRO:HD3	1.98	0.42
1:D:384:HIS:O	1:D:386:PRO:HD3	2.20	0.42
1:A:69:SER:OG	1:A:346:ILE:HD13	2.19	0.42
1:C:268:PHE:HE2	1:D:306:ARG:HD3	1.85	0.42
1:C:247:HIS:HE1	1:C:275:LYS:O	2.03	0.42
1:C:389:VAL:C	1:C:391:ALA:H	2.23	0.42
1:A:197:VAL:O	1:A:201:VAL:HG23	2.20	0.42
1:C:110:VAL:HB	1:C:190:ILE:HB	2.02	0.42
1:C:349:SER:CB	1:C:352:MSE:HE3	2.50	0.42
1:B:361:GLN:HG2	1:B:462:PHE:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:PHE:HZ	1:A:348:VAL:HG22	1.84	0.42
1:B:71:MSE:CB	1:B:249:ILE:HD11	2.44	0.42
1:A:88:MSE:HE2	1:A:88:MSE:N	2.34	0.42
1:A:317:TRP:CZ2	1:A:479:ILE:HD11	2.55	0.42
1:C:131:MSE:HE3	1:C:192:ILE:HG12	2.02	0.42
1:D:421:LYS:HG2	1:D:422:ASN:N	2.34	0.42
1:D:162:VAL:HA	1:D:163:PRO:HD3	1.96	0.42
1:C:139:HIS:O	1:C:140:GLN:CB	2.66	0.41
1:B:88:MSE:HG2	3:B:688:HOH:O	2.19	0.41
1:D:196:ASP:O	1:D:200:VAL:HG22	2.20	0.41
1:D:101:ILE:HG12	1:D:235:ILE:HG22	2.00	0.41
1:A:141:ARG:NE	1:A:182:LYS:HZ1	2.18	0.41
1:A:183:THR:HG22	1:A:256:GLU:OE2	2.19	0.41
1:C:23:GLU:HA	1:C:35:PHE:O	2.20	0.41
1:A:230:ILE:HG12	1:A:231:ASP:N	2.34	0.41
1:B:375:LEU:O	1:B:454:GLU:CG	2.59	0.41
1:A:258:ARG:NH1	1:A:259:ASP:OD2	2.54	0.41
1:A:141:ARG:NH1	1:A:258:ARG:NH2	2.68	0.41
1:D:462:PHE:CD2	1:D:469:MSE:HE3	2.55	0.41
1:C:407:MSE:HE2	1:C:415:PRO:HG2	2.01	0.41
1:B:408:ILE:HD13	3:B:756:HOH:O	2.19	0.41
1:C:162:VAL:O	1:C:181:PRO:HD2	2.19	0.41
1:C:247:HIS:CE1	1:C:275:LYS:O	2.74	0.41
1:C:460:PHE:CZ	1:C:476:MSE:HE1	2.56	0.41
1:D:128:GLU:O	1:D:129:ALA:HB2	2.20	0.41
1:A:323:VAL:HG22	1:A:324:SER:O	2.20	0.41
1:A:251:GLN:NE2	1:A:274:GLY:H	2.01	0.41
1:D:286:ILE:N	1:D:286:ILE:HD12	2.36	0.41
1:C:162:VAL:HA	1:C:163:PRO:HD3	1.89	0.41
1:C:182:LYS:CD	1:C:256:GLU:OE1	2.69	0.41
1:D:66:PRO:HG3	1:D:338:ARG:HG2	2.01	0.41
1:B:227:VAL:HA	1:B:228:PRO:HD3	1.87	0.41
1:B:378:GLU:O	1:B:435:TYR:HE1	2.04	0.41
1:A:190:ILE:HG22	1:A:191:ARG:N	2.35	0.41
1:C:98:GLN:OE1	1:C:409:ILE:HD11	2.21	0.41
1:B:167:LYS:HE3	1:C:25:VAL:O	2.19	0.41
1:A:123:ILE:O	1:A:210:THR:HA	2.21	0.41
1:B:468:LYS:HB2	1:B:468:LYS:NZ	2.26	0.41
1:A:101:ILE:HD12	1:A:344:GLU:C	2.40	0.41
1:C:240:LEU:HD11	1:C:284:LYS:HD2	2.03	0.41
1:B:445:ASN:OD1	1:B:445:ASN:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:TRP:CZ3	1:D:476:MSE:HB3	2.56	0.41
1:B:451:ASN:N	1:B:451:ASN:HD22	2.18	0.41
1:B:407:MSE:HB3	1:B:415:PRO:HB3	2.02	0.41
1:B:454:GLU:CD	1:B:454:GLU:C	2.80	0.41
1:A:56:ARG:HD3	1:A:265:GLN:CB	2.50	0.41
1:B:468:LYS:NZ	1:B:468:LYS:CB	2.83	0.41
1:B:335:LEU:HD12	1:B:338:ARG:HH12	1.86	0.41
1:B:382:LYS:CB	1:B:481:LEU:HD11	2.49	0.41
1:C:312:TRP:CZ3	1:C:476:MSE:HB3	2.56	0.41
1:D:242:TYR:O	1:D:246:ILE:HG12	2.21	0.41
1:A:390:PRO:HB3	1:A:466:THR:OG1	2.21	0.41
1:B:422:ASN:HB2	1:B:445:ASN:OD1	2.21	0.41
1:D:434:TYR:O	1:D:447:TRP:HA	2.21	0.41
1:A:384:HIS:O	1:A:386:PRO:HD3	2.21	0.41
1:C:140:GLN:O	1:C:140:GLN:CG	2.56	0.41
1:A:397:THR:O	1:A:416:ASP:HB2	2.21	0.41
1:A:362:ARG:NH1	1:A:469:MSE:HE2	2.35	0.41
1:B:116:LEU:HD11	1:B:161:ILE:HG22	2.02	0.41
1:A:72:GLU:HB3	1:A:234:HIS:O	2.21	0.41
1:C:88:MSE:HG2	3:C:614:HOH:O	2.20	0.41
1:A:174:LYS:HB3	1:A:174:LYS:HZ3	1.85	0.41
1:A:162:VAL:HA	1:A:163:PRO:HD3	1.93	0.41
1:C:422:ASN:HA	3:C:771:HOH:O	2.20	0.41
1:B:166:GLU:HG2	1:B:169:LYS:HD3	2.03	0.41
1:B:259:ASP:O	1:B:263:MSE:HG2	2.20	0.41
1:A:471:ASP:O	1:A:472:LYS:HB2	2.21	0.41
1:B:398:THR:O	1:B:457:PHE:HB2	2.21	0.40
1:A:111:ILE:HG22	1:A:112:GLY:N	2.36	0.40
1:A:205:VAL:HG23	1:A:206:PRO:CD	2.52	0.40
1:A:174:LYS:CB	1:A:174:LYS:NZ	2.84	0.40
1:C:282:GLU:HG3	1:C:283:GLN:H	1.85	0.40
1:A:292:LYS:HD2	1:B:28:SER:HB3	2.02	0.40
1:A:434:TYR:CD1	1:A:440:VAL:HG21	2.56	0.40
1:B:399:VAL:HB	1:B:447:TRP:CZ2	2.56	0.40
1:D:88:MSE:HE1	1:D:114:TRP:CZ3	2.57	0.40
1:D:89:GLY:HA2	1:D:225:ALA:O	2.21	0.40
1:D:185:VAL:H	1:D:253:ASN:ND2	2.16	0.40
1:D:135:MSE:HE2	1:D:188:GLY:HA2	2.03	0.40
1:D:137:ASP:C	1:D:137:ASP:OD1	2.60	0.40
1:B:208:ILE:O	1:B:224:VAL:HG23	2.20	0.40
1:A:151:PRO:HD2	1:A:159:TYR:OH	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PHE:CZ	1:B:367:TYR:HB3	2.57	0.40
1:B:247:HIS:CG	1:B:277:PHE:HB2	2.57	0.40
1:A:334:GLU:HB3	1:A:337:GLU:HB2	2.04	0.40
1:A:66:PRO:HG2	1:A:338:ARG:CG	2.40	0.40
1:B:74:LEU:HB2	1:B:113:THR:HG21	2.03	0.40
1:B:140:GLN:HE22	1:B:346:ILE:HD12	1.86	0.40
1:B:433:VAL:HG23	1:B:446:ASN:HA	2.02	0.40
1:B:23:GLU:O	1:B:24:THR:HG23	2.21	0.40
1:B:436:GLY:O	1:B:448:VAL:HG23	2.20	0.40
1:B:435:TYR:CZ	1:B:437:PRO:HD2	2.55	0.40
1:C:66:PRO:O	1:C:342:PHE:CE2	2.74	0.40
1:C:62:LEU:CD1	1:C:297:MSE:HE2	2.45	0.40
1:A:141:ARG:CZ	1:A:327:GLN:OE1	2.70	0.40
1:A:194:GLU:HA	1:A:195:PRO:HD3	1.84	0.40
1:C:126:LEU:HA	1:C:127:PRO:HD3	1.85	0.40
1:C:481:LEU:HD22	1:C:482:VAL:N	2.35	0.40
1:B:378:GLU:OE1	1:B:379:HIS:CE1	2.74	0.40
1:C:142:VAL:CG2	1:C:348:VAL:HG13	2.52	0.40
1:C:140:GLN:OE1	1:C:342:PHE:CD1	2.75	0.40
1:D:116:LEU:HD11	1:D:181:PRO:HG3	2.04	0.40
1:B:363:TYR:CD1	1:B:363:TYR:N	2.89	0.40
1:B:477:GLY:HA3	3:B:635:HOH:O	2.20	0.40
1:A:311:TYR:OH	1:A:469:MSE:HE3	2.21	0.40
1:B:470:PHE:CG	1:B:472:LYS:HE3	2.57	0.40
1:A:389:VAL:HA	1:A:390:PRO:HD3	1.88	0.40
1:D:37:SER:O	1:D:38:ASP:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	458/483 (95%)	436 (95%)	20 (4%)	2 (0%)	39	37
1	B	460/483 (95%)	428 (93%)	26 (6%)	6 (1%)	15	9
1	C	458/483 (95%)	435 (95%)	18 (4%)	5 (1%)	17	11
1	D	458/483 (95%)	432 (94%)	23 (5%)	3 (1%)	26	21
All	All	1834/1932 (95%)	1731 (94%)	87 (5%)	16 (1%)	21	15

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	419	SER
1	B	452	PRO
1	C	334	GLU
1	A	334	GLU
1	B	437	PRO
1	C	147	SER
1	C	197	VAL
1	B	454	GLU
1	B	463	TYR
1	D	334	GLU
1	B	215	ASP
1	D	214	ALA
1	A	147	SER
1	C	390	PRO
1	D	147	SER
1	C	330	GLU

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	405/408 (99%)	389 (96%)	16 (4%)	38	38
1	B	407/408 (100%)	393 (97%)	14 (3%)	44	45
1	C	405/408 (99%)	393 (97%)	12 (3%)	48	51
1	D	405/408 (99%)	397 (98%)	8 (2%)	63	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1622/1632 (99%)	1572 (97%)	50 (3%)	47 50

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	33	LEU
1	A	39	PHE
1	A	72	GLU
1	A	94	LEU
1	A	101	ILE
1	A	104	ASN
1	A	117	GLU
1	A	145	ASP
1	A	166	GLU
1	A	174	LYS
1	A	308	THR
1	A	348	VAL
1	A	363	TYR
1	A	408	ILE
1	A	469	MSE
1	B	22	GLN
1	B	29	ARG
1	B	104	ASN
1	B	145	ASP
1	B	172	ASN
1	B	187	TYR
1	B	229	GLU
1	B	269	LEU
1	B	408	ILE
1	B	452	PRO
1	B	454	GLU
1	B	461	ARG
1	B	468	LYS
1	B	469	MSE
1	C	95	LYS
1	C	134	MSE
1	C	145	ASP
1	C	169	LYS
1	C	198	ASP
1	C	306	ARG
1	C	329	SER

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Mol	Chain	Res	Type
1	C	342	PHE
1	C	347	THR
1	C	424	LYS
1	C	469	MSE
1	C	476	MSE
1	D	33	LEU
1	D	101	ILE
1	D	145	ASP
1	D	176	TYR
1	D	196	ASP
1	D	230	ILE
1	D	405	ARG
1	D	469	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	ASN
1	A	50	ASN
1	A	59	GLN
1	A	87	GLN
1	A	104	ASN
1	A	125	ASN
1	A	172	ASN
1	A	207	ASN
1	A	234	HIS
1	A	247	HIS
1	A	248	GLN
1	A	251	GLN
1	A	253	ASN
1	A	426	ASN
1	A	445	ASN
1	B	22	GLN
1	B	59	GLN
1	B	98	GLN
1	B	104	ASN
1	B	139	HIS
1	B	172	ASN
1	B	226	GLN
1	B	234	HIS
1	B	247	HIS
1	B	248	GLN

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Mol	Chain	Res	Type
1	B	251	GLN
1	B	253	ASN
1	B	368	GLN
1	B	379	HIS
1	B	451	ASN
1	C	59	GLN
1	C	92	ASN
1	C	96	GLN
1	C	125	ASN
1	C	203	GLN
1	C	226	GLN
1	C	234	HIS
1	C	247	HIS
1	C	248	GLN
1	C	251	GLN
1	C	253	ASN
1	C	361	GLN
1	C	368	GLN
1	C	379	HIS
1	C	422	ASN
1	D	59	GLN
1	D	75	ASN
1	D	125	ASN
1	D	140	GLN
1	D	234	HIS
1	D	247	HIS
1	D	251	GLN
1	D	253	ASN
1	D	379	HIS
1	D	404	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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	446/483 (92%)	0.47	29 (6%)	22	29	10, 24, 45, 55	0
1	B	448/483 (92%)	0.69	48 (10%)	8	11	8, 24, 51, 68	0
1	C	446/483 (92%)	0.49	28 (6%)	23	31	8, 24, 45, 64	0
1	D	446/483 (92%)	0.38	18 (4%)	42	51	10, 21, 40, 59	0
All	All	1786/1932 (92%)	0.51	123 (6%)	20	27	8, 23, 45, 68	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	447	TRP	13.4
1	B	437	PRO	8.6
1	B	463	TYR	6.7
1	B	474	TRP	6.6
1	A	482	VAL	6.5
1	B	481	LEU	6.0
1	B	443	TYR	5.9
1	B	452	PRO	5.8
1	D	440	VAL	5.6
1	B	454	GLU	5.6
1	B	435	TYR	5.5
1	B	451	ASN	5.4
1	C	342	PHE	5.0
1	B	470	PHE	5.0
1	D	215	ASP	5.0
1	B	428	ASP	4.9
1	A	24	THR	4.6
1	B	215	ASP	4.6
1	B	457	PHE	4.4
1	C	215	ASP	4.3
1	B	420	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	411	ASP	4.1
1	B	441	LYS	4.0
1	A	230	ILE	4.0
1	C	482	VAL	4.0
1	B	482	VAL	3.9
1	B	456	TRP	3.7
1	D	447	TRP	3.7
1	A	215	ASP	3.6
1	C	341	TRP	3.5
1	C	443	TYR	3.5
1	D	441	LYS	3.5
1	B	388	ASN	3.4
1	D	442	GLY	3.4
1	A	341	TRP	3.3
1	D	482	VAL	3.2
1	B	374	TRP	3.2
1	B	415	PRO	3.2
1	A	481	LEU	3.2
1	B	453	GLY	3.1
1	C	330	GLU	3.1
1	B	483	LYS	3.0
1	A	431	ILE	3.0
1	A	441	LYS	3.0
1	B	203	GLN	3.0
1	B	439	PRO	3.0
1	B	169	LYS	2.9
1	A	359	PHE	2.9
1	D	388	ASN	2.9
1	A	190	ILE	2.8
1	B	408	ILE	2.8
1	B	424	LYS	2.8
1	B	426	ASN	2.8
1	A	198	ASP	2.8
1	A	167	LYS	2.8
1	A	356	ILE	2.8
1	D	443	TYR	2.8
1	B	421	LYS	2.8
1	A	479	ILE	2.7
1	C	439	PRO	2.7
1	B	460	PHE	2.7
1	C	346	ILE	2.7
1	A	169	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	438	LYS	2.7
1	C	278	ASN	2.7
1	D	481	LEU	2.7
1	C	422	ASN	2.6
1	B	448	VAL	2.6
1	C	428	ASP	2.6
1	C	199	ARG	2.6
1	A	197	VAL	2.6
1	D	101	ILE	2.5
1	C	103	ALA	2.5
1	B	230	ILE	2.5
1	B	198	ASP	2.4
1	B	216	GLY	2.4
1	B	166	GLU	2.4
1	B	170	ASP	2.4
1	C	426	ASN	2.4
1	C	197	VAL	2.3
1	B	65	ILE	2.3
1	A	39	PHE	2.3
1	C	427	SER	2.3
1	D	214	ALA	2.3
1	C	479	ILE	2.3
1	C	169	LYS	2.3
1	A	171	LEU	2.3
1	A	196	ASP	2.3
1	B	431	ILE	2.3
1	B	449	GLN	2.3
1	A	278	ASN	2.3
1	C	167	LYS	2.3
1	D	411	ASP	2.3
1	C	436	GLY	2.2
1	D	216	GLY	2.2
1	D	453	GLY	2.2
1	B	432	ASP	2.2
1	C	356	ILE	2.2
1	D	231	ASP	2.2
1	B	172	ASN	2.2
1	C	268	PHE	2.2
1	D	438	LYS	2.2
1	C	343	TYR	2.2
1	D	124	ILE	2.2
1	C	431	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	475	THR	2.1
1	B	235	ILE	2.1
1	A	440	VAL	2.1
1	A	453	GLY	2.1
1	A	229	GLU	2.1
1	A	66	PRO	2.1
1	A	298	ALA	2.1
1	A	340	ALA	2.1
1	B	466	THR	2.1
1	D	155	LYS	2.1
1	C	216	GLY	2.1
1	B	62	LEU	2.1
1	A	166	GLU	2.1
1	C	24	THR	2.0
1	C	388	ASN	2.0
1	A	23	GLU	2.0
1	A	65	ILE	2.0
1	C	198	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	MG	D	502	1/1	0.97	0.43	18.16	20,20,20,20	0
2	MG	A	502	1/1	0.97	0.42	13.30	16,16,16,16	0
2	MG	B	502	1/1	0.96	0.44	7.00	21,21,21,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	B	501	1/1	0.98	0.20	4.75	18,18,18,18	0
2	MG	A	501	1/1	0.99	0.17	1.14	16,16,16,16	0
2	MG	C	501	1/1	0.99	0.13	0.45	13,13,13,13	0
2	MG	D	501	1/1	0.98	0.13	0.34	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.