



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:55 am GMT

PDB ID : 3KFK
Title : Crystal structures of a group II chaperonin from *Methanococcus maripaludis*
Authors : Pereira, J.H.; Ralston, C.Y.; Douglas, N.; Meyer, D.; Knee, K.M.; Goulet, D.R.; King, J.A.; Frydman, J.; Adams, P.D.
Deposited on : 2009-10-27
Resolution : 6.00 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

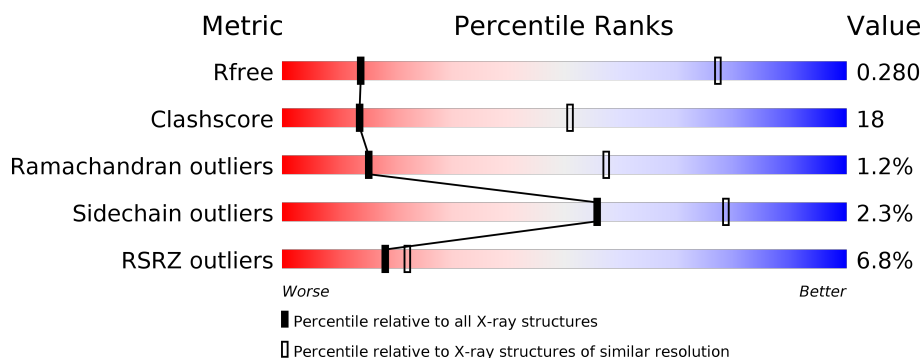
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 6.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1085 (8.30-3.70)
Clashscore	112137	1017 (8.20-3.80)
Ramachandran outliers	110173	1001 (8.20-3.72)
Sidechain outliers	110143	1085 (8.30-3.70)
RSRZ outliers	101464	1094 (8.30-3.70)

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	521	<div> <div>5%</div> <div> <div></div> <div>75%</div> <div>17%</div> <div>• 7%</div> </div> </div>
1	B	521	<div> <div>6%</div> <div> <div></div> <div>69%</div> <div>23%</div> <div>• 7%</div> </div> </div>
1	C	521	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>20%</div> <div>• 7%</div> </div> </div>
1	D	521	<div> <div>11%</div> <div> <div></div> <div>75%</div> <div>15%</div> <div>• 7%</div> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AGS	D	544	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14619 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 Chaperonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3629	2249	631	725	24			
1	B	487	Total	C	N	O	S	0	0	0
			3629	2249	631	725	24			
1	C	487	Total	C	N	O	S	0	0	0
			3629	2249	631	725	24			
1	D	484	Total	C	N	O	S	0	0	0
			3608	2235	627	722	24			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	DELETION	UNP Q877G8
A	?	-	LYS	DELETION	UNP Q877G8
A	?	-	GLU	DELETION	UNP Q877G8
A	?	-	THR	DELETION	UNP Q877G8
A	?	-	ASP	DELETION	UNP Q877G8
A	?	-	ALA	DELETION	UNP Q877G8
A	?	-	GLU	DELETION	UNP Q877G8
A	?	-	ILE	DELETION	UNP Q877G8
A	?	-	ARG	DELETION	UNP Q877G8
A	?	-	ILE	DELETION	UNP Q877G8
A	?	-	THR	DELETION	UNP Q877G8
A	?	-	ASP	DELETION	UNP Q877G8
A	?	-	PRO	DELETION	UNP Q877G8
A	?	-	LYS	DELETION	UNP Q877G8
A	?	-	LEU	DELETION	UNP Q877G8
A	?	-	MET	DELETION	UNP Q877G8
A	?	-	GLU	DELETION	UNP Q877G8
A	?	-	PHE	DELETION	UNP Q877G8
A	?	-	ILE	DELETION	UNP Q877G8
A	264	THR	GLN	ENGINEERED MUTATION	UNP Q877G8
A	265	ALA	GLU	ENGINEERED MUTATION	UNP Q877G8

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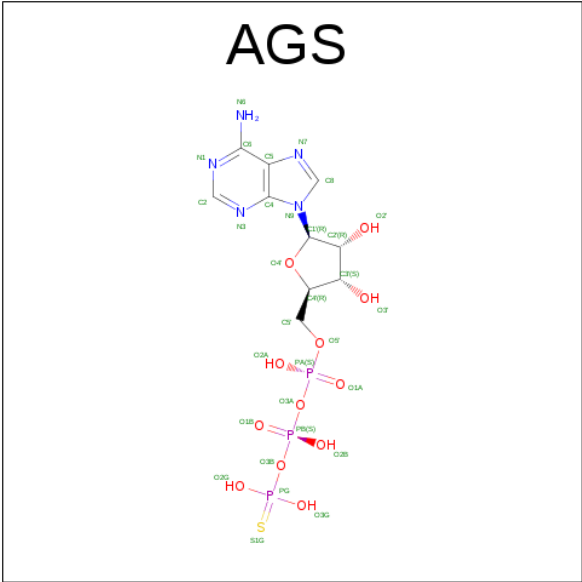
Chain	Residue	Modelled	Actual	Comment	Reference
A	266	SER	GLU	ENGINEERED MUTATION	UNP Q877G8
A	267	GLU	LYS	ENGINEERED MUTATION	UNP Q877G8
B	?	-	ILE	DELETION	UNP Q877G8
B	?	-	LYS	DELETION	UNP Q877G8
B	?	-	GLU	DELETION	UNP Q877G8
B	?	-	THR	DELETION	UNP Q877G8
B	?	-	ASP	DELETION	UNP Q877G8
B	?	-	ALA	DELETION	UNP Q877G8
B	?	-	GLU	DELETION	UNP Q877G8
B	?	-	ILE	DELETION	UNP Q877G8
B	?	-	ARG	DELETION	UNP Q877G8
B	?	-	ILE	DELETION	UNP Q877G8
B	?	-	THR	DELETION	UNP Q877G8
B	?	-	ASP	DELETION	UNP Q877G8
B	?	-	PRO	DELETION	UNP Q877G8
B	?	-	LYS	DELETION	UNP Q877G8
B	?	-	LEU	DELETION	UNP Q877G8
B	?	-	MET	DELETION	UNP Q877G8
B	?	-	GLU	DELETION	UNP Q877G8
B	?	-	PHE	DELETION	UNP Q877G8
B	?	-	ILE	DELETION	UNP Q877G8
B	264	THR	GLN	ENGINEERED MUTATION	UNP Q877G8
B	265	ALA	GLU	ENGINEERED MUTATION	UNP Q877G8
B	266	SER	GLU	ENGINEERED MUTATION	UNP Q877G8
B	267	GLU	LYS	ENGINEERED MUTATION	UNP Q877G8
C	?	-	ILE	DELETION	UNP Q877G8
C	?	-	LYS	DELETION	UNP Q877G8
C	?	-	GLU	DELETION	UNP Q877G8
C	?	-	THR	DELETION	UNP Q877G8
C	?	-	ASP	DELETION	UNP Q877G8
C	?	-	ALA	DELETION	UNP Q877G8
C	?	-	GLU	DELETION	UNP Q877G8
C	?	-	ILE	DELETION	UNP Q877G8
C	?	-	ARG	DELETION	UNP Q877G8
C	?	-	ILE	DELETION	UNP Q877G8
C	?	-	THR	DELETION	UNP Q877G8
C	?	-	ASP	DELETION	UNP Q877G8
C	?	-	PRO	DELETION	UNP Q877G8
C	?	-	LYS	DELETION	UNP Q877G8
C	?	-	LEU	DELETION	UNP Q877G8
C	?	-	MET	DELETION	UNP Q877G8
C	?	-	GLU	DELETION	UNP Q877G8

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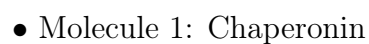
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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	PHE	DELETION	UNP Q877G8
C	?	-	ILE	DELETION	UNP Q877G8
C	264	THR	GLN	ENGINEERED MUTATION	UNP Q877G8
C	265	ALA	GLU	ENGINEERED MUTATION	UNP Q877G8
C	266	SER	GLU	ENGINEERED MUTATION	UNP Q877G8
C	267	GLU	LYS	ENGINEERED MUTATION	UNP Q877G8
D	?	-	ILE	DELETION	UNP Q877G8
D	?	-	LYS	DELETION	UNP Q877G8
D	?	-	GLU	DELETION	UNP Q877G8
D	?	-	THR	DELETION	UNP Q877G8
D	?	-	ASP	DELETION	UNP Q877G8
D	?	-	ALA	DELETION	UNP Q877G8
D	?	-	GLU	DELETION	UNP Q877G8
D	?	-	ILE	DELETION	UNP Q877G8
D	?	-	ARG	DELETION	UNP Q877G8
D	?	-	ILE	DELETION	UNP Q877G8
D	?	-	THR	DELETION	UNP Q877G8
D	?	-	ASP	DELETION	UNP Q877G8
D	?	-	PRO	DELETION	UNP Q877G8
D	?	-	LYS	DELETION	UNP Q877G8
D	?	-	LEU	DELETION	UNP Q877G8
D	?	-	MET	DELETION	UNP Q877G8
D	?	-	GLU	DELETION	UNP Q877G8
D	?	-	PHE	DELETION	UNP Q877G8
D	?	-	ILE	DELETION	UNP Q877G8
D	264	THR	GLN	ENGINEERED MUTATION	UNP Q877G8
D	265	ALA	GLU	ENGINEERED MUTATION	UNP Q877G8
D	266	SER	GLU	ENGINEERED MUTATION	UNP Q877G8
D	267	GLU	LYS	ENGINEERED MUTATION	UNP Q877G8

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	150.53Å 209.53Å 266.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.56 – 6.00 58.56 – 6.00	Depositor EDS
% Data completeness (in resolution range)	95.1 (58.56-6.00) 95.6 (58.56-6.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 6.17Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_241)	Depositor
R, R_{free}	0.241 , 0.270 0.243 , 0.280	Depositor DCC
R_{free} test set	492 reflections (4.77%)	DCC
Wilson B-factor (Å ²)	342.4	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 386.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	14619	wwPDB-VP
Average B, all atoms (Å ²)	555.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.31	0/3649	0.46	2/4911 (0.0%)
1	B	0.31	0/3649	0.46	2/4911 (0.0%)
1	C	0.32	0/3649	0.47	2/4911 (0.0%)
1	D	0.31	0/3627	0.46	2/4881 (0.0%)
All	All	0.31	0/14574	0.46	8/19614 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	3
1	C	0	4
1	D	0	4
All	All	0	13

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	263	GLU	N-CA-C	6.25	127.89	111.00
1	C	263	GLU	N-CA-C	6.17	127.64	111.00
1	D	263	GLU	N-CA-C	6.12	127.51	111.00
1	B	263	GLU	N-CA-C	6.10	127.48	111.00
1	A	240	GLU	N-CA-C	5.84	126.77	111.00
1	C	240	GLU	N-CA-C	5.81	126.70	111.00
1	D	240	GLU	N-CA-C	5.67	126.32	111.00
1	B	240	GLU	N-CA-C	5.39	125.54	111.00

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	355	PHE	Peptide
1	A	398	GLY	Peptide
1	B	211	GLY	Peptide
1	B	358	GLU	Peptide
1	B	398	GLY	Peptide
1	C	143	GLY	Peptide
1	C	210	LYS	Peptide
1	C	397	ASP	Peptide
1	C	398	GLY	Peptide
1	D	357	GLU	Peptide
1	D	360	LYS	Peptide
1	D	361	HIS	Peptide
1	D	398	GLY	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3629	0	3764	131	2
1	B	3629	0	3762	204	0
1	C	3629	0	3762	151	1
1	D	3608	0	3736	99	1
2	A	31	0	12	5	0
2	B	31	0	12	5	0
2	C	31	0	12	6	0
2	D	31	0	12	11	0
All	All	14619	0	15072	525	2

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 18.

All (525) 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:210:LYS:CB	1:A:358:GLU:H	1.13	1.53
2:D:544:AGS:PG	2:D:544:AGS:S1G	1.49	1.49
2:B:544:AGS:S1G	2:B:544:AGS:PG	1.49	1.48
2:A:544:AGS:PG	2:A:544:AGS:S1G	1.49	1.47
2:C:544:AGS:PG	2:C:544:AGS:S1G	1.49	1.47
1:A:210:LYS:HB2	1:A:358:GLU:N	1.17	1.42
1:A:210:LYS:CB	1:A:358:GLU:N	1.78	1.32
1:C:142:VAL:CG2	1:C:149:ILE:HG21	1.61	1.29
1:C:142:VAL:HG21	1:C:149:ILE:CG2	1.66	1.24
1:D:263:GLU:CB	1:D:269:LEU:HD11	1.68	1.24
1:B:390:VAL:HG12	1:B:491:PRO:CG	1.69	1.22
1:C:196:GLU:OE1	1:C:316:LYS:HE2	1.40	1.22
1:C:263:GLU:CB	1:C:269:LEU:HD11	1.71	1.20
1:B:490:GLU:OE1	1:B:495:LYS:HE2	1.42	1.20
1:B:349:SER:HB2	1:B:370:ARG:NH2	1.55	1.19
1:C:399:ARG:HD2	1:C:492:LEU:HD22	1.26	1.18
1:A:218:ARG:NH1	1:A:225:LYS:HE2	1.59	1.18
1:A:263:GLU:CB	1:A:269:LEU:HD11	1.72	1.17
1:A:210:LYS:CD	1:A:358:GLU:HA	1.77	1.15
1:B:194:LYS:HB2	1:B:316:LYS:CE	1.80	1.12
1:C:142:VAL:HG22	1:C:149:ILE:HD13	1.22	1.12
1:B:341:GLY:HA3	1:B:358:GLU:HG2	1.16	1.11
1:B:348:ILE:HG23	1:B:370:ARG:NH2	1.64	1.11
1:C:142:VAL:HG11	1:C:149:ILE:HB	1.20	1.10
1:A:210:LYS:HD2	1:A:358:GLU:HA	1.13	1.10
1:A:218:ARG:HH12	1:A:225:LYS:HE2	1.06	1.09
1:B:42:LYS:HB3	1:C:118:THR:HG21	1.30	1.09
1:A:210:LYS:HB2	1:A:358:GLU:CA	1.83	1.09
1:B:390:VAL:CG1	1:B:491:PRO:HG2	1.81	1.09
1:B:348:ILE:HG23	1:B:370:ARG:HH22	0.95	1.07
1:B:341:GLY:HA3	1:B:358:GLU:CG	1.82	1.07
1:B:69:SER:HB3	1:C:11:ASN:ND2	1.69	1.07
1:A:210:LYS:CB	1:A:358:GLU:CA	2.30	1.07
1:D:269:LEU:HD23	1:D:294:ALA:CB	1.83	1.07
1:B:194:LYS:HB2	1:B:316:LYS:HE3	1.14	1.06
1:C:269:LEU:HD23	1:C:294:ALA:HB2	1.06	1.06
1:C:269:LEU:HD23	1:C:294:ALA:CB	1.85	1.05
1:A:269:LEU:HD23	1:A:294:ALA:CB	1.86	1.05
1:B:42:LYS:HD2	1:C:118:THR:HB	1.36	1.03
1:D:269:LEU:HD23	1:D:294:ALA:HB2	1.03	1.03
1:A:210:LYS:HB3	1:A:358:GLU:N	1.71	1.03
1:C:42:LYS:HD2	1:D:118:THR:HB	1.35	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:LYS:HB3	1:B:359:CYS:HB3	1.40	1.01
1:A:269:LEU:HD23	1:A:294:ALA:HB2	1.05	1.01
1:A:194:LYS:HD2	1:A:316:LYS:CD	1.92	0.99
1:B:399:ARG:HD2	1:B:492:LEU:HD22	1.45	0.98
1:B:142:VAL:HG21	1:B:153:ILE:HD11	1.46	0.97
1:C:209:ILE:CG2	1:C:211:GLY:CA	2.41	0.97
1:A:399:ARG:HD2	1:A:492:LEU:HD22	1.45	0.97
1:B:399:ARG:HD2	1:B:492:LEU:CD2	1.94	0.97
1:D:360:LYS:O	1:D:362:PRO:HG3	1.64	0.96
1:A:194:LYS:CD	1:A:316:LYS:HD3	1.94	0.96
1:B:194:LYS:N	1:B:316:LYS:HZ2	1.64	0.96
1:C:142:VAL:HG13	1:C:149:ILE:HD12	1.48	0.96
1:B:240:GLU:O	1:B:269:LEU:HD11	1.66	0.96
1:C:142:VAL:CG2	1:C:149:ILE:HD13	1.97	0.95
1:B:194:LYS:N	1:B:316:LYS:NZ	2.15	0.94
1:A:42:LYS:HE3	1:B:118:THR:HB	1.50	0.93
1:A:207:GLU:HG3	1:A:209:ILE:HD13	1.48	0.93
1:A:194:LYS:HD2	1:A:316:LYS:HD3	0.98	0.93
1:B:69:SER:HB3	1:C:11:ASN:HD22	1.27	0.93
1:B:390:VAL:HG12	1:B:491:PRO:HG2	0.94	0.93
1:C:399:ARG:HD2	1:C:492:LEU:CD2	2.00	0.92
1:B:194:LYS:CB	1:B:316:LYS:HE3	1.99	0.92
1:C:209:ILE:HG22	1:C:211:GLY:CA	2.00	0.92
1:C:142:VAL:HG11	1:C:149:ILE:CB	1.98	0.92
1:D:269:LEU:CD2	1:D:294:ALA:HB2	1.98	0.92
1:C:490:GLU:OE1	1:C:495:LYS:HE2	1.68	0.92
1:C:209:ILE:HG23	1:C:211:GLY:HA3	1.52	0.91
1:B:341:GLY:CA	1:B:358:GLU:HG2	1.99	0.91
1:B:210:LYS:HB3	1:B:359:CYS:CB	2.02	0.90
1:A:269:LEU:CD2	1:A:294:ALA:HB2	1.99	0.90
1:B:348:ILE:CG2	1:B:370:ARG:HH22	1.84	0.90
1:B:142:VAL:HB	1:B:394:THR:CG2	2.02	0.89
1:C:209:ILE:CG2	1:C:211:GLY:C	2.40	0.89
1:A:210:LYS:CG	1:A:358:GLU:HA	2.02	0.89
1:D:357:GLU:HG2	1:D:358:GLU:HB2	1.55	0.89
1:B:490:GLU:OE1	1:B:495:LYS:CE	2.21	0.88
1:C:156:THR:HG21	1:C:489:VAL:O	1.74	0.88
1:B:142:VAL:HG12	1:B:142:VAL:O	1.72	0.87
1:C:142:VAL:CG1	1:C:149:ILE:HB	2.04	0.87
1:D:196:GLU:OE2	1:D:213:LEU:HB2	1.75	0.87
1:B:156:THR:HG21	1:B:489:VAL:N	1.89	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:SER:HB2	1:B:370:ARG:HH21	1.37	0.86
1:A:210:LYS:HD2	1:A:358:GLU:CA	2.04	0.86
1:A:449:GLY:HA2	1:B:116:HIS:CG	2.11	0.85
1:D:399:ARG:HD2	1:D:492:LEU:HD22	1.56	0.85
1:A:399:ARG:HD2	1:A:492:LEU:CD2	2.05	0.85
1:B:349:SER:HB2	1:B:370:ARG:CZ	2.05	0.85
1:B:50:ASP:HA	1:C:518:ALA:CB	2.07	0.85
1:B:50:ASP:HA	1:C:518:ALA:HB3	1.59	0.85
1:B:218:ARG:NH1	1:B:223:MET:O	2.08	0.85
1:A:207:GLU:HG3	1:A:209:ILE:CD1	2.07	0.85
1:A:343:VAL:HA	1:A:355:PHE:O	1.77	0.85
1:C:209:ILE:HG22	1:C:211:GLY:N	1.92	0.84
1:B:341:GLY:HA3	1:B:358:GLU:CB	2.06	0.84
1:B:390:VAL:CG1	1:B:491:PRO:CG	2.46	0.84
1:C:213:LEU:HD22	1:C:368:LEU:CD2	2.06	0.84
1:B:50:ASP:CA	1:C:518:ALA:HB3	2.07	0.84
1:C:213:LEU:HD22	1:C:368:LEU:HD21	1.58	0.84
1:C:449:GLY:HA2	1:D:116:HIS:CG	2.13	0.83
1:A:42:LYS:HB3	1:B:118:THR:HG21	1.61	0.83
1:C:269:LEU:CD2	1:C:294:ALA:HB2	2.01	0.82
1:A:211:GLY:CA	1:A:357:GLU:HA	2.08	0.82
1:B:42:LYS:HD2	1:C:118:THR:CB	2.09	0.82
1:C:209:ILE:CG2	1:C:211:GLY:HA3	2.08	0.82
1:B:194:LYS:HE3	1:B:313:ASP:OD1	1.80	0.82
1:A:218:ARG:NH1	1:A:225:LYS:CE	2.43	0.81
1:B:49:VAL:O	1:C:518:ALA:N	2.11	0.81
1:B:50:ASP:C	1:C:518:ALA:HB3	2.00	0.81
1:A:218:ARG:NH2	1:A:225:LYS:HZ1	1.79	0.81
1:D:360:LYS:O	1:D:362:PRO:HD3	1.79	0.81
1:B:48:LEU:CD1	1:C:516:ILE:HD12	2.11	0.81
1:D:263:GLU:CB	1:D:269:LEU:CD1	2.54	0.81
1:D:342:LEU:HB2	1:D:358:GLU:CG	2.10	0.80
1:D:360:LYS:O	1:D:362:PRO:CG	2.28	0.80
1:B:46:LYS:NZ	1:C:514:ASP:HB2	1.96	0.80
1:D:357:GLU:HB2	1:D:366:THR:OG1	1.81	0.80
1:A:218:ARG:NH2	1:A:225:LYS:NZ	2.30	0.80
1:D:342:LEU:CB	1:D:358:GLU:CB	2.59	0.80
1:C:276:ILE:HA	1:C:332:LEU:HD23	1.64	0.80
1:D:341:GLY:HA3	1:D:358:GLU:O	1.81	0.79
1:C:263:GLU:CB	1:C:269:LEU:CD1	2.57	0.79
1:A:263:GLU:CB	1:A:269:LEU:CD1	2.57	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:VAL:N	1:B:398:GLY:O	2.17	0.78
1:A:341:GLY:HA3	1:A:358:GLU:O	1.83	0.78
1:A:210:LYS:CB	1:A:358:GLU:HA	2.11	0.78
1:B:263:GLU:CB	1:B:269:LEU:HD21	2.13	0.78
1:A:42:LYS:CE	1:B:118:THR:HB	2.14	0.77
2:C:544:AGS:S1G	2:C:544:AGS:O3G	2.42	0.77
2:A:544:AGS:O3G	2:A:544:AGS:S1G	2.42	0.77
1:D:360:LYS:O	1:D:362:PRO:CD	2.31	0.77
1:A:218:ARG:CZ	1:A:225:LYS:NZ	2.47	0.77
1:B:46:LYS:HZ2	1:C:514:ASP:HB2	1.51	0.76
1:D:198:LYS:HE3	1:D:213:LEU:CD2	2.14	0.76
1:A:211:GLY:N	1:A:357:GLU:HA	2.01	0.76
1:A:209:ILE:HD11	1:A:368:LEU:HB3	1.66	0.75
1:A:211:GLY:HA3	1:A:357:GLU:HA	1.67	0.75
1:D:399:ARG:HD2	1:D:492:LEU:CD2	2.15	0.75
1:B:357:GLU:O	1:B:358:GLU:CB	2.33	0.75
1:A:42:LYS:HE3	1:B:118:THR:CB	2.16	0.74
1:A:218:ARG:CZ	1:A:225:LYS:HE2	2.17	0.74
1:A:210:LYS:HB2	1:A:358:GLU:H	0.58	0.74
1:B:358:GLU:HA	1:B:358:GLU:OE2	1.88	0.73
2:B:544:AGS:S1G	2:B:544:AGS:O3G	2.42	0.73
1:C:60:ASP:HA	2:C:544:AGS:S1G	2.28	0.73
2:D:544:AGS:S1G	2:D:544:AGS:O3G	2.42	0.73
1:C:156:THR:CG2	1:C:489:VAL:O	2.37	0.73
1:B:213:LEU:CD2	1:B:368:LEU:HD13	2.19	0.72
1:D:342:LEU:HB2	1:D:358:GLU:CB	2.17	0.72
1:D:142:VAL:N	1:D:398:GLY:O	2.18	0.72
1:B:390:VAL:HG12	1:B:491:PRO:CD	2.19	0.72
1:A:142:VAL:HG22	1:A:149:ILE:HG21	1.72	0.71
1:D:342:LEU:CB	1:D:358:GLU:HB3	2.20	0.71
1:D:342:LEU:HD13	1:D:358:GLU:HG2	1.73	0.71
1:B:156:THR:HG21	1:B:489:VAL:H	1.54	0.71
1:D:342:LEU:HB3	1:D:358:GLU:CB	2.21	0.71
1:B:42:LYS:HB3	1:C:118:THR:CG2	2.15	0.71
1:C:209:ILE:HG22	1:C:211:GLY:O	1.91	0.71
1:B:69:SER:CB	1:C:11:ASN:ND2	2.51	0.71
1:D:342:LEU:N	1:D:358:GLU:HB3	2.05	0.71
1:A:390:VAL:HG12	1:A:491:PRO:HG2	1.73	0.70
1:C:42:LYS:HB3	1:D:118:THR:HG21	1.72	0.70
1:C:142:VAL:HG22	1:C:149:ILE:CD1	2.11	0.70
1:D:342:LEU:HB2	1:D:358:GLU:HB3	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:GLU:O	1:B:269:LEU:CD1	2.39	0.70
1:A:209:ILE:HD12	1:A:368:LEU:HB2	1.72	0.70
1:B:358:GLU:CD	1:B:358:GLU:O	2.30	0.70
1:D:358:GLU:O	1:D:359:CYS:SG	2.49	0.70
1:A:209:ILE:CD1	1:A:368:LEU:HB2	2.21	0.70
1:B:341:GLY:HA3	1:B:358:GLU:HB2	1.72	0.69
1:B:358:GLU:OE2	1:B:358:GLU:CA	2.39	0.69
1:C:209:ILE:HG22	1:C:211:GLY:C	2.06	0.69
1:D:342:LEU:CB	1:D:358:GLU:CG	2.70	0.69
1:D:342:LEU:CB	1:D:358:GLU:HG2	2.22	0.69
1:B:193:ILE:C	1:B:316:LYS:HZ1	1.96	0.68
1:A:210:LYS:CA	1:A:358:GLU:H	2.00	0.68
1:C:209:ILE:HG21	1:C:211:GLY:C	2.14	0.68
1:B:42:LYS:CD	1:C:118:THR:HB	2.19	0.67
1:A:447:ASN:O	1:B:116:HIS:CE1	2.47	0.67
1:A:218:ARG:CZ	1:A:225:LYS:CE	2.73	0.67
1:A:210:LYS:CG	1:A:358:GLU:CA	2.69	0.67
1:A:209:ILE:HD11	1:A:368:LEU:CB	2.25	0.66
1:B:156:THR:CG2	1:B:489:VAL:H	2.08	0.66
1:C:156:THR:CB	1:C:489:VAL:O	2.44	0.66
1:B:349:SER:CB	1:B:370:ARG:HH21	2.09	0.66
1:A:342:LEU:HB3	1:A:357:GLU:HG3	1.78	0.65
1:B:341:GLY:CA	1:B:358:GLU:CG	2.67	0.65
1:C:156:THR:HG21	1:C:489:VAL:C	2.16	0.65
1:B:46:LYS:NZ	1:C:514:ASP:CB	2.60	0.65
1:A:209:ILE:CD1	1:A:368:LEU:CB	2.74	0.65
1:B:60:ASP:HA	2:B:544:AGS:S1G	2.37	0.65
1:C:209:ILE:CG2	1:C:211:GLY:O	2.43	0.65
1:D:390:VAL:HG12	1:D:491:PRO:HG2	1.78	0.65
1:C:393:CYS:SG	1:C:493:ARG:NH1	2.70	0.64
1:B:397:ASP:HB3	1:B:399:ARG:HG3	1.79	0.64
1:C:399:ARG:CD	1:C:492:LEU:HD22	2.16	0.64
1:A:218:ARG:CZ	1:A:225:LYS:HZ3	2.10	0.64
1:A:142:VAL:CG2	1:A:149:ILE:HG21	2.28	0.64
1:A:142:VAL:HG12	1:A:142:VAL:O	1.97	0.64
1:A:218:ARG:NH2	1:A:225:LYS:CE	2.61	0.64
1:B:194:LYS:N	1:B:316:LYS:HZ1	1.96	0.64
1:D:142:VAL:O	1:D:142:VAL:HG12	1.98	0.64
1:D:360:LYS:HD2	1:D:361:HIS:H	1.63	0.63
1:B:209:ILE:HD13	1:B:213:LEU:HD13	1.81	0.63
1:B:156:THR:HG21	1:B:489:VAL:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:ASN:O	1:C:116:HIS:CE1	2.51	0.63
1:B:341:GLY:CA	1:B:358:GLU:CB	2.77	0.63
1:B:399:ARG:HD2	1:B:492:LEU:HD23	1.78	0.63
1:C:142:VAL:CG1	1:C:146:ASP:HB3	2.29	0.63
1:C:327:THR:O	1:C:328:ASN:HB2	1.99	0.63
1:D:357:GLU:CG	1:D:358:GLU:HB2	2.29	0.62
1:C:142:VAL:HG13	1:C:149:ILE:CD1	2.25	0.62
1:A:210:LYS:HG2	1:A:359:CYS:N	2.15	0.62
1:A:449:GLY:HA2	1:B:116:HIS:CD2	2.33	0.62
1:B:46:LYS:HD2	1:C:514:ASP:HB3	1.80	0.62
1:A:210:LYS:HB3	1:A:358:GLU:CA	2.22	0.62
1:A:449:GLY:HA2	1:B:116:HIS:CB	2.30	0.62
1:A:46:LYS:NZ	1:B:514:ASP:CB	2.63	0.62
1:A:46:LYS:NZ	1:B:514:ASP:HB2	2.15	0.61
1:C:209:ILE:HG22	1:C:211:GLY:H	1.64	0.61
1:A:210:LYS:C	1:A:357:GLU:HA	2.21	0.61
1:D:342:LEU:HB3	1:D:358:GLU:HB2	1.82	0.61
1:B:153:ILE:HG12	1:B:400:ILE:HG21	1.83	0.61
1:C:449:GLY:HA2	1:D:116:HIS:CB	2.30	0.61
1:B:142:VAL:O	1:B:143:GLY:C	2.38	0.61
1:B:37:SER:OG	1:C:513:ASP:OD2	2.19	0.61
1:A:211:GLY:HA3	1:A:357:GLU:CA	2.31	0.60
1:C:213:LEU:HD22	1:C:368:LEU:HD22	1.83	0.60
1:C:95:THR:HG23	2:C:544:AGS:O2B	2.01	0.60
1:D:357:GLU:HG3	1:D:358:GLU:OE1	2.01	0.60
1:C:470:CYS:SG	1:C:484:CYS:N	2.75	0.60
1:B:198:LYS:NZ	1:B:215:ASP:OD2	2.33	0.60
1:D:374:GLU:HA	1:D:377:ILE:HD12	1.83	0.60
1:B:218:ARG:NH2	1:B:221:ALA:O	2.35	0.60
1:B:341:GLY:H	1:B:358:GLU:HB3	1.67	0.60
1:B:156:THR:CG2	1:B:489:VAL:O	2.51	0.59
1:C:390:VAL:HG12	1:C:491:PRO:HG2	1.83	0.59
1:B:156:THR:CG2	1:B:489:VAL:N	2.65	0.59
1:B:390:VAL:CG1	1:B:491:PRO:CD	2.78	0.59
1:C:153:ILE:HG12	1:C:400:ILE:HG21	1.84	0.59
1:B:210:LYS:CB	1:B:359:CYS:CB	2.77	0.59
1:B:194:LYS:HD3	1:B:366:THR:HG23	1.85	0.58
1:A:37:SER:OG	1:B:513:ASP:OD2	2.15	0.58
1:C:328:ASN:O	1:C:330:LYS:N	2.37	0.58
1:A:374:GLU:HA	1:A:377:ILE:HD12	1.85	0.58
1:B:46:LYS:CD	1:C:514:ASP:HB3	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:GLU:O	1:B:358:GLU:HB3	2.03	0.58
1:B:194:LYS:CB	1:B:316:LYS:CE	2.67	0.58
1:A:142:VAL:O	1:A:143:GLY:C	2.42	0.58
1:B:194:LYS:HD3	1:B:366:THR:CG2	2.34	0.58
1:B:357:GLU:O	1:B:358:GLU:HB2	2.03	0.58
1:A:213:LEU:HD22	1:A:368:LEU:HD11	1.86	0.58
1:B:193:ILE:C	1:B:316:LYS:NZ	2.56	0.58
1:B:25:ILE:HG23	1:B:104:LEU:HB3	1.86	0.57
1:B:213:LEU:HD22	1:B:368:LEU:HD13	1.86	0.57
1:B:374:GLU:HA	1:B:377:ILE:HD12	1.86	0.57
1:B:194:LYS:CE	1:B:313:ASP:OD1	2.51	0.57
1:C:374:GLU:HA	1:C:377:ILE:HD12	1.86	0.57
1:B:390:VAL:CB	1:B:491:PRO:CG	2.81	0.57
1:A:173:ILE:HG23	1:A:208:LEU:HB2	1.86	0.57
1:B:341:GLY:CA	1:B:358:GLU:HB2	2.34	0.57
1:C:25:ILE:HG23	1:C:104:LEU:HB3	1.86	0.57
1:C:42:LYS:HD2	1:D:118:THR:CB	2.24	0.57
1:B:46:LYS:HZ2	1:C:514:ASP:CB	2.16	0.57
1:B:194:LYS:H	1:B:316:LYS:HZ2	1.47	0.57
1:B:358:GLU:O	1:B:358:GLU:CG	2.52	0.57
1:B:142:VAL:CB	1:B:394:THR:CG2	2.81	0.56
1:A:470:CYS:HG	1:A:484:CYS:HG	0.58	0.56
1:A:95:THR:HG23	2:A:544:AGS:O2B	2.04	0.56
1:C:142:VAL:HG11	1:C:149:ILE:CG2	2.35	0.56
1:A:60:ASP:HA	2:A:544:AGS:S1G	2.45	0.56
1:C:42:LYS:HB3	1:D:118:THR:CG2	2.35	0.56
1:B:48:LEU:HD12	1:C:516:ILE:HD12	1.85	0.56
1:A:449:GLY:CA	1:B:116:HIS:CG	2.87	0.56
1:D:135:LEU:HD23	1:D:138:ILE:HD11	1.87	0.56
1:B:48:LEU:HD11	1:C:516:ILE:HD12	1.89	0.55
1:D:490:GLU:OE2	2:D:544:AGS:C2'	2.54	0.55
1:B:142:VAL:HG21	1:B:153:ILE:CD1	2.31	0.55
1:B:368:LEU:HD23	1:B:370:ARG:NH1	2.20	0.55
1:A:25:ILE:HG23	1:A:104:LEU:HB3	1.89	0.55
1:B:390:VAL:HB	1:B:491:PRO:HG3	1.89	0.55
1:A:194:LYS:HE3	1:A:316:LYS:HA	1.89	0.55
1:A:349:SER:HB2	1:A:370:ARG:HH22	1.71	0.55
1:C:48:LEU:HD11	1:C:64:ILE:HG23	1.89	0.55
1:A:447:ASN:O	1:B:116:HIS:HE1	1.87	0.54
1:B:368:LEU:HD21	1:B:370:ARG:CZ	2.36	0.54
1:A:349:SER:HB2	1:A:370:ARG:NH2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:LYS:O	1:B:359:CYS:HB2	2.07	0.54
1:B:194:LYS:CA	1:B:316:LYS:NZ	2.71	0.54
1:D:342:LEU:CD1	1:D:358:GLU:HG2	2.36	0.54
1:A:210:LYS:HD2	1:A:358:GLU:HG2	1.89	0.54
1:C:393:CYS:SG	1:C:493:ARG:CZ	2.96	0.54
1:B:142:VAL:HG11	1:B:394:THR:HG21	1.89	0.54
1:D:269:LEU:HD22	1:D:294:ALA:N	2.23	0.54
1:B:344:GLU:OE1	1:B:346:ARG:NE	2.24	0.54
1:B:196:GLU:OE2	1:B:215:ASP:HB2	2.09	0.53
1:B:368:LEU:CD2	1:B:370:ARG:NH1	2.71	0.53
1:C:269:LEU:HD22	1:C:294:ALA:N	2.23	0.53
1:D:25:ILE:HG23	1:D:104:LEU:HB3	1.90	0.53
1:D:95:THR:HG23	2:D:544:AGS:O2B	2.07	0.53
1:C:37:SER:OG	1:D:513:ASP:OD2	2.26	0.53
1:B:142:VAL:HG22	1:B:149:ILE:HG21	1.91	0.53
1:D:119:ILE:HG21	1:D:425:ARG:HB3	1.90	0.53
1:D:48:LEU:HD11	1:D:64:ILE:HG23	1.91	0.53
1:A:239:ILE:HD12	1:A:290:ILE:HG12	1.91	0.53
1:B:156:THR:HB	1:B:489:VAL:O	2.08	0.53
1:C:142:VAL:CG2	1:C:149:ILE:CD1	2.79	0.53
1:A:211:GLY:HA3	1:A:356:VAL:C	2.30	0.52
1:D:490:GLU:OE2	2:D:544:AGS:H3'	2.09	0.52
1:B:213:LEU:HD23	1:B:368:LEU:HD13	1.89	0.52
1:C:341:GLY:HA3	1:C:358:GLU:O	2.09	0.52
1:D:142:VAL:O	1:D:143:GLY:C	2.48	0.52
1:B:349:SER:CB	1:B:370:ARG:NH2	2.48	0.52
1:A:46:LYS:NZ	1:B:514:ASP:HB3	2.25	0.52
1:A:320:ALA:HA	1:A:364:ALA:CB	2.40	0.52
1:B:46:LYS:HZ3	1:C:514:ASP:HB2	1.74	0.52
1:B:142:VAL:CG1	1:B:142:VAL:O	2.46	0.52
1:B:50:ASP:HA	1:C:518:ALA:HB2	1.89	0.52
1:C:46:LYS:NZ	1:D:514:ASP:HB2	2.25	0.52
1:D:195:ILE:HG23	1:D:369:ILE:HD12	1.93	0.52
1:C:142:VAL:HG12	1:C:146:ASP:HB3	1.91	0.51
1:C:156:THR:HB	1:C:489:VAL:O	2.10	0.51
2:C:544:AGS:S1G	2:C:544:AGS:O3B	2.58	0.51
1:C:449:GLY:CA	1:D:116:HIS:CG	2.92	0.51
1:D:216:LYS:HD2	1:D:307:ARG:O	2.10	0.51
2:D:544:AGS:O3B	2:D:544:AGS:S1G	2.58	0.51
1:B:142:VAL:HB	1:B:394:THR:HG23	1.88	0.51
1:C:46:LYS:NZ	1:D:514:ASP:CB	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ILE:HG21	1:A:425:ARG:HB3	1.91	0.51
1:C:446:GLU:O	1:D:116:HIS:NE2	2.44	0.51
1:B:369:ILE:HD13	1:B:381:ALA:HA	1.92	0.51
2:B:544:AGS:O3B	2:B:544:AGS:S1G	2.58	0.51
1:B:195:ILE:HG23	1:B:369:ILE:HD12	1.92	0.51
1:A:218:ARG:HH22	1:A:225:LYS:CE	2.24	0.51
1:B:156:THR:HG21	1:B:489:VAL:C	2.30	0.51
1:A:46:LYS:HZ2	1:B:514:ASP:CB	2.23	0.50
1:C:195:ILE:HG23	1:C:369:ILE:HD12	1.92	0.50
1:D:239:ILE:HD12	1:D:290:ILE:HG12	1.93	0.50
1:A:235:LEU:HD12	1:A:284:LEU:HD11	1.92	0.50
1:C:398:GLY:O	1:C:399:ARG:HG3	2.12	0.50
1:C:239:ILE:HD12	1:C:290:ILE:HG12	1.92	0.50
1:C:210:LYS:HG2	1:C:362:PRO:HG2	1.93	0.50
1:D:404:GLY:HA2	2:D:544:AGS:N3	2.27	0.50
1:B:216:LYS:HD2	1:B:307:ARG:O	2.12	0.50
1:A:369:ILE:HD13	1:A:381:ALA:HA	1.92	0.50
1:B:390:VAL:CB	1:B:491:PRO:HG2	2.38	0.50
1:A:195:ILE:HG23	1:A:369:ILE:HD12	1.92	0.50
1:C:269:LEU:CD2	1:C:294:ALA:N	2.75	0.50
1:C:399:ARG:CD	1:C:492:LEU:CD2	2.81	0.50
1:D:360:LYS:CD	1:D:361:HIS:H	2.24	0.49
1:B:141:GLU:HA	1:B:398:GLY:O	2.11	0.49
1:B:194:LYS:HB2	1:B:316:LYS:CD	2.40	0.49
1:A:182:VAL:HG22	1:A:188:VAL:HG22	1.94	0.49
1:B:156:THR:CB	1:B:489:VAL:O	2.61	0.49
1:D:369:ILE:HD13	1:D:381:ALA:HA	1.94	0.49
1:B:210:LYS:CB	1:B:359:CYS:HB2	2.42	0.49
1:B:393:CYS:SG	1:B:493:ARG:CZ	3.00	0.49
1:A:269:LEU:HD22	1:A:294:ALA:N	2.27	0.49
1:C:206:THR:HG22	1:C:370:ARG:H	1.78	0.49
1:A:320:ALA:HA	1:A:364:ALA:HB3	1.94	0.49
1:C:135:LEU:HD23	1:C:138:ILE:HD11	1.95	0.49
1:C:119:ILE:HG21	1:C:425:ARG:HB3	1.95	0.49
1:A:211:GLY:HA3	1:A:356:VAL:O	2.13	0.49
1:D:269:LEU:CD2	1:D:294:ALA:N	2.76	0.49
2:A:544:AGS:O3B	2:A:544:AGS:S1G	2.58	0.49
1:C:182:VAL:HG22	1:C:188:VAL:HG22	1.95	0.49
1:B:182:VAL:HG22	1:B:188:VAL:HG22	1.95	0.49
1:B:173:ILE:HG23	1:B:208:LEU:HB2	1.95	0.49
1:D:173:ILE:HG23	1:D:208:LEU:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:LEU:HD12	1:B:284:LEU:HD11	1.95	0.48
1:C:216:LYS:HD2	1:C:307:ARG:O	2.13	0.48
1:C:369:ILE:HD13	1:C:381:ALA:HA	1.93	0.48
1:A:46:LYS:HZ3	1:B:514:ASP:CB	2.24	0.48
1:B:119:ILE:HG21	1:B:425:ARG:HB3	1.94	0.48
1:B:240:GLU:C	1:B:269:LEU:HD11	2.33	0.48
1:C:46:LYS:HZ2	1:D:514:ASP:CB	2.27	0.48
1:A:213:LEU:HD11	1:A:355:PHE:CZ	2.49	0.48
1:D:206:THR:HG22	1:D:370:ARG:H	1.78	0.48
1:A:118:THR:HA	1:A:121:VAL:HG12	1.95	0.48
1:B:142:VAL:CG1	1:B:394:THR:HG21	2.43	0.48
1:D:198:LYS:HD3	1:D:198:LYS:HA	1.57	0.48
1:A:449:GLY:HA2	1:B:116:HIS:HB2	1.96	0.48
1:C:142:VAL:CG1	1:C:149:ILE:HD12	2.32	0.48
1:A:48:LEU:HD11	1:A:64:ILE:HG23	1.95	0.48
1:B:118:THR:HA	1:B:121:VAL:HG12	1.95	0.48
1:A:206:THR:HG22	1:A:370:ARG:H	1.79	0.48
1:A:455:ILE:HG21	1:A:473:LEU:HD13	1.96	0.48
1:B:206:THR:HG22	1:B:370:ARG:H	1.78	0.48
1:C:142:VAL:CG1	1:C:149:ILE:CD1	2.90	0.48
1:B:135:LEU:HD23	1:B:138:ILE:HD11	1.96	0.47
1:B:239:ILE:HD12	1:B:290:ILE:HG12	1.95	0.47
1:B:210:LYS:C	1:B:359:CYS:SG	2.92	0.47
1:D:360:LYS:CD	1:D:361:HIS:N	2.77	0.47
1:B:142:VAL:HB	1:B:394:THR:HG22	1.92	0.47
1:C:490:GLU:CD	1:C:495:LYS:HE2	2.32	0.47
1:D:223:MET:HB3	1:D:304:VAL:HG22	1.95	0.47
1:D:404:GLY:CA	2:D:544:AGS:N3	2.78	0.47
1:A:135:LEU:HD23	1:A:138:ILE:HD11	1.96	0.47
1:C:173:ILE:HG23	1:C:208:LEU:HB2	1.96	0.47
1:B:341:GLY:H	1:B:358:GLU:CB	2.28	0.47
1:C:142:VAL:HG21	1:C:149:ILE:HG21	0.69	0.47
1:C:118:THR:HA	1:C:121:VAL:HG12	1.97	0.47
1:C:327:THR:O	1:C:328:ASN:CB	2.61	0.47
1:B:91:ASP:HB2	1:B:386:ASP:OD2	2.15	0.47
1:C:449:GLY:HA2	1:D:116:HIS:CD2	2.48	0.47
1:C:142:VAL:CG1	1:C:149:ILE:CB	2.78	0.47
1:B:143:GLY:O	1:B:145:GLN:N	2.48	0.46
1:D:182:VAL:HG22	1:D:188:VAL:HG22	1.97	0.46
1:B:11:ASN:HA	1:B:12:MET:HA	1.50	0.46
1:B:215:ASP:HA	1:B:353:MET:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:THR:HG23	2:B:544:AGS:O2B	2.15	0.46
1:D:403:GLY:HA3	2:D:544:AGS:O2'	2.15	0.46
1:A:341:GLY:CA	1:A:358:GLU:O	2.60	0.46
1:D:470:CYS:SG	1:D:484:CYS:N	2.89	0.46
1:A:184:ASP:HA	1:A:185:GLU:HA	1.61	0.46
1:A:356:VAL:O	1:A:357:GLU:HB3	2.16	0.46
1:B:399:ARG:CD	1:B:492:LEU:CD2	2.83	0.46
1:B:48:LEU:HD11	1:B:64:ILE:HG23	1.97	0.46
1:A:209:ILE:HG13	1:A:368:LEU:H	1.80	0.46
1:B:347:LYS:HG2	1:B:352:SER:HB3	1.97	0.46
1:C:184:ASP:HA	1:C:185:GLU:HA	1.60	0.46
1:D:11:ASN:HA	1:D:12:MET:HA	1.51	0.46
1:D:141:GLU:HA	1:D:398:GLY:O	2.15	0.46
1:A:150:LEU:HD22	1:A:391:VAL:HG13	1.97	0.46
1:B:49:VAL:O	1:C:518:ALA:CB	2.64	0.46
1:C:404:GLY:HA2	2:C:544:AGS:N3	2.30	0.46
1:A:216:LYS:HD2	1:A:307:ARG:O	2.16	0.46
1:D:468:ASN:O	1:D:469:LYS:HB3	2.16	0.46
1:D:490:GLU:CD	2:D:544:AGS:O2'	2.54	0.46
1:A:344:GLU:N	1:A:355:PHE:O	2.46	0.45
1:A:470:CYS:HG	1:A:484:CYS:CB	2.22	0.45
1:C:210:LYS:HG2	1:C:362:PRO:CG	2.47	0.45
1:B:142:VAL:HG23	1:B:400:ILE:HG12	1.98	0.45
1:C:213:LEU:CD2	1:C:368:LEU:HD21	2.40	0.45
1:C:209:ILE:HG21	1:C:211:GLY:O	2.15	0.45
1:C:357:GLU:O	1:C:358:GLU:HB2	2.16	0.45
1:C:401:VAL:HB	1:C:407:THR:HG21	1.99	0.45
1:B:449:GLY:HA2	1:C:116:HIS:HB2	1.97	0.45
1:A:213:LEU:HD22	1:A:368:LEU:CD1	2.46	0.45
1:B:194:LYS:CA	1:B:316:LYS:HZ2	2.28	0.45
1:C:150:LEU:HD22	1:C:391:VAL:HG13	1.99	0.45
1:C:69:SER:HB3	1:D:11:ASN:ND2	2.32	0.45
1:B:150:LEU:HD22	1:B:391:VAL:HG13	1.98	0.45
1:B:455:ILE:HG21	1:B:473:LEU:HD13	1.98	0.45
1:D:401:VAL:HB	1:D:407:THR:HG21	1.97	0.45
1:B:198:LYS:HA	1:B:198:LYS:HD3	1.59	0.45
1:D:215:ASP:HA	1:D:353:MET:HG2	1.98	0.45
1:B:46:LYS:HZ3	1:C:514:ASP:CB	2.28	0.44
1:D:150:LEU:HD22	1:D:391:VAL:HG13	1.99	0.44
1:D:118:THR:HA	1:D:121:VAL:HG12	1.99	0.44
1:A:46:LYS:HZ2	1:B:514:ASP:HB2	1.79	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:347:LYS:HG2	1:D:352:SER:HB3	1.98	0.44
1:A:401:VAL:HB	1:A:407:THR:HG21	1.98	0.44
1:C:269:LEU:CD2	1:C:294:ALA:H	2.31	0.44
1:B:449:GLY:HA2	1:C:116:HIS:CB	2.47	0.44
1:B:48:LEU:HA	1:C:516:ILE:HB	2.00	0.44
1:B:470:CYS:SG	1:B:484:CYS:N	2.91	0.44
1:D:342:LEU:HB3	1:D:358:GLU:HG2	1.98	0.44
1:B:449:GLY:HA2	1:C:116:HIS:CG	2.52	0.44
1:A:470:CYS:SG	1:A:484:CYS:N	2.91	0.43
1:B:341:GLY:N	1:B:358:GLU:CB	2.81	0.43
1:D:490:GLU:OE2	2:D:544:AGS:C3'	2.66	0.43
1:C:447:ASN:O	1:D:118:THR:HG21	2.19	0.43
1:D:470:CYS:SG	1:D:484:CYS:CB	3.05	0.43
1:A:228:THR:HG22	1:A:229:ASP:OD1	2.18	0.43
1:A:440:ILE:HB	1:A:441:PRO:HD3	2.00	0.43
1:C:46:LYS:NZ	1:D:514:ASP:HB3	2.34	0.43
1:D:235:LEU:HD12	1:D:284:LEU:HD11	1.99	0.43
1:B:142:VAL:CB	1:B:394:THR:HG21	2.48	0.43
1:B:48:LEU:HG	1:C:516:ILE:CD1	2.48	0.43
1:A:470:CYS:SG	1:A:484:CYS:CB	3.05	0.43
1:B:144:ALA:HB1	1:B:395:ILE:HG23	2.01	0.43
1:A:228:THR:HG22	1:A:229:ASP:CG	2.39	0.43
1:A:37:SER:CB	1:B:513:ASP:OD2	2.67	0.43
1:A:213:LEU:HD11	1:A:355:PHE:CE1	2.54	0.42
1:D:184:ASP:HA	1:D:185:GLU:HA	1.61	0.42
1:B:390:VAL:CB	1:B:491:PRO:HG3	2.47	0.42
1:A:449:GLY:CA	1:B:116:HIS:CB	2.95	0.42
1:C:79:ILE:HG22	1:C:79:ILE:O	2.20	0.42
1:B:358:GLU:OE2	1:B:358:GLU:C	2.58	0.42
1:B:194:LYS:CB	1:B:316:LYS:HZ2	2.32	0.42
1:A:207:GLU:O	1:A:209:ILE:HG12	2.20	0.42
1:B:324:ASN:HB2	1:B:336:ASP:HB3	2.00	0.42
1:B:440:ILE:HB	1:B:441:PRO:HD3	2.01	0.42
1:C:11:ASN:HA	1:C:12:MET:HA	1.51	0.42
1:B:184:ASP:HA	1:B:185:GLU:HA	1.61	0.42
1:B:399:ARG:CD	1:B:492:LEU:HD23	2.47	0.42
1:B:194:LYS:CB	1:B:316:LYS:NZ	2.83	0.42
1:B:236:ASN:HB2	1:B:325:VAL:HG12	2.02	0.42
1:D:130:LYS:HA	1:D:133:GLU:HG2	2.01	0.42
1:D:455:ILE:HG21	1:D:473:LEU:HD13	2.01	0.42
1:A:210:LYS:HD2	1:A:358:GLU:CG	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:440:ILE:HB	1:D:441:PRO:HD3	2.02	0.41
1:B:390:VAL:HB	1:B:491:PRO:CG	2.48	0.41
1:B:79:ILE:O	1:B:79:ILE:HG22	2.20	0.41
1:C:440:ILE:HB	1:C:441:PRO:HD3	2.02	0.41
1:C:468:ASN:O	1:C:469:LYS:HB3	2.20	0.41
1:A:72:HIS:HA	1:A:73:PRO:HD3	1.94	0.41
1:D:79:ILE:HG22	1:D:79:ILE:O	2.20	0.41
1:A:419:ALA:HA	1:A:422:ILE:HD12	2.02	0.41
1:B:194:LYS:HB2	1:B:316:LYS:NZ	2.33	0.41
1:B:419:ALA:HA	1:B:422:ILE:HD12	2.03	0.41
1:C:398:GLY:O	1:C:399:ARG:CG	2.69	0.41
1:C:390:VAL:CG1	1:C:491:PRO:HG2	2.49	0.41
1:A:342:LEU:N	1:A:357:GLU:O	2.52	0.41
1:B:192:LEU:O	1:B:316:LYS:NZ	2.47	0.41
1:B:401:VAL:HB	1:B:407:THR:HG21	2.02	0.41
1:C:185:GLU:HA	1:C:186:GLY:HA2	1.94	0.41
1:C:347:LYS:HG2	1:C:352:SER:HB3	2.02	0.41
1:C:449:GLY:HA2	1:D:116:HIS:HB2	2.02	0.41
1:A:210:LYS:HB3	1:A:358:GLU:C	2.40	0.41
1:C:69:SER:HB3	1:D:11:ASN:HD22	1.86	0.41
1:C:72:HIS:HA	1:C:73:PRO:HD3	1.96	0.41
1:D:269:LEU:CD2	1:D:294:ALA:H	2.33	0.41
1:A:207:GLU:HG3	1:A:209:ILE:HD11	1.96	0.40
1:B:468:ASN:O	1:B:469:LYS:HB3	2.22	0.40
1:A:269:LEU:HD21	1:A:291:ASP:HB3	2.02	0.40
1:C:419:ALA:HA	1:C:422:ILE:HD12	2.04	0.40
1:C:455:ILE:HG21	1:C:473:LEU:HD13	2.03	0.40
1:A:347:LYS:HG2	1:A:352:SER:HB3	2.03	0.40
1:B:49:VAL:HB	1:C:517:ALA:HA	2.04	0.40
1:D:361:HIS:HA	1:D:362:PRO:HD3	1.80	0.40
1:A:269:LEU:CD2	1:A:294:ALA:N	2.84	0.40
1:C:398:GLY:O	1:C:399:ARG:CB	2.70	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LYS:CB	1:C:335:GLN:CG[8_444]	2.14	0.06
1:A:518:ALA:N	1:D:49:VAL:O[2_545]	2.15	0.05

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	485/521 (93%)	454 (94%)	26 (5%)	5 (1%)	18	61
1	B	485/521 (93%)	449 (93%)	30 (6%)	6 (1%)	15	57
1	C	485/521 (93%)	446 (92%)	34 (7%)	5 (1%)	18	61
1	D	480/521 (92%)	442 (92%)	31 (6%)	7 (2%)	12	53
All	All	1935/2084 (93%)	1791 (93%)	121 (6%)	23 (1%)	15	57

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	358	GLU
1	C	328	ASN
1	C	329	ILE
1	D	358	GLU
1	D	361	HIS
1	A	17	GLY
1	A	143	GLY
1	B	17	GLY
1	B	143	GLY
1	C	17	GLY
1	D	17	GLY
1	D	143	GLY
1	C	465	SER
1	D	465	SER
1	A	465	SER
1	B	465	SER
1	A	201	ALA
1	A	358	GLU
1	B	201	ALA
1	B	263	GLU
1	C	201	ALA
1	D	201	ALA
1	D	362	PRO

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	388/413 (94%)	376 (97%)	12 (3%)	45	71
1	B	388/413 (94%)	379 (98%)	9 (2%)	56	78
1	C	388/413 (94%)	383 (99%)	5 (1%)	73	87
1	D	386/413 (94%)	377 (98%)	9 (2%)	56	78
All	All	1550/1652 (94%)	1515 (98%)	35 (2%)	56	78

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

Mol	Chain	Res	Type
1	A	37	SER
1	A	39	LEU
1	A	209	ILE
1	A	210	LYS
1	A	216	LYS
1	A	225	LYS
1	A	229	ASP
1	A	300	LYS
1	A	327	THR
1	A	356	VAL
1	A	358	GLU
1	A	386	ASP
1	B	45	ASP
1	B	216	LYS
1	B	218	ARG
1	B	225	LYS
1	B	327	THR
1	B	335	GLN
1	B	342	LEU
1	B	349	SER
1	B	358	GLU
1	C	194	LYS
1	C	216	LYS
1	C	327	THR

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Mol	Chain	Res	Type
1	C	342	LEU
1	C	453	ILE
1	D	45	ASP
1	D	137	THR
1	D	196	GLU
1	D	198	LYS
1	D	216	LYS
1	D	227	VAL
1	D	327	THR
1	D	357	GLU
1	D	490	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	11	ASN
1	B	129	GLN
1	C	11	ASN
1	C	129	GLN
1	D	11	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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	AGS	A	544	-	26,33,33	4.38	4 (15%)	22,52,52	1.08	0
2	AGS	B	544	-	26,33,33	4.37	4 (15%)	22,52,52	1.07	0
2	AGS	C	544	-	26,33,33	4.38	4 (15%)	22,52,52	1.07	0
2	AGS	D	544	-	26,33,33	4.38	4 (15%)	22,52,52	1.07	0

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	AGS	A	544	-	-	0/17/38/38	0/3/3/3
2	AGS	B	544	-	-	0/17/38/38	0/3/3/3
2	AGS	C	544	-	-	0/17/38/38	0/3/3/3
2	AGS	D	544	-	-	0/17/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	544	AGS	PG-S1G	-21.54	1.49	1.90
2	A	544	AGS	PG-S1G	-21.54	1.49	1.90
2	D	544	AGS	PG-S1G	-21.53	1.49	1.90
2	B	544	AGS	PG-S1G	-21.50	1.49	1.90
2	A	544	AGS	C4-N3	2.07	1.38	1.35
2	D	544	AGS	C4-N3	2.10	1.38	1.35
2	B	544	AGS	C4-N3	2.11	1.38	1.35
2	C	544	AGS	C4-N3	2.11	1.38	1.35
2	B	544	AGS	C2-N3	2.30	1.36	1.32
2	D	544	AGS	C2-N3	2.36	1.36	1.32
2	A	544	AGS	C2-N3	2.39	1.36	1.32
2	C	544	AGS	C2-N3	2.40	1.36	1.32
2	B	544	AGS	O4'-C1'	2.47	1.44	1.41
2	D	544	AGS	O4'-C1'	2.51	1.44	1.41
2	C	544	AGS	O4'-C1'	2.52	1.44	1.41
2	A	544	AGS	O4'-C1'	2.56	1.44	1.41

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	544	AGS	5	0
2	B	544	AGS	5	0
2	C	544	AGS	6	0
2	D	544	AGS	11	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	487/521 (93%)	0.37	25 (5%)	29	31	283, 526, 830, 912	0
1	B	487/521 (93%)	0.36	31 (6%)	20	23	246, 522, 794, 846	0
1	C	487/521 (93%)	0.29	21 (4%)	36	35	294, 527, 844, 901	0
1	D	484/521 (92%)	0.63	55 (11%)	6	12	303, 528, 839, 939	0
All	All	1945/2084 (93%)	0.41	132 (6%)	18	22	246, 526, 824, 939	0

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	349	SER	8.2
1	D	226	LYS	7.3
1	D	188	VAL	6.8
1	D	344	GLU	6.8
1	D	327	THR	6.6
1	D	343	VAL	6.6
1	D	225	LYS	6.5
1	D	355	PHE	6.0
1	D	326	ILE	5.6
1	C	144	ALA	5.6
1	D	395	ILE	5.4
1	D	354	ILE	4.8
1	B	237	CYS	4.8
1	B	327	THR	4.7
1	C	343	VAL	4.7
1	D	237	CYS	4.6
1	C	344	GLU	4.4
1	D	356	VAL	4.3
1	D	345	GLU	4.3
1	B	328	ASN	4.3
1	D	394	THR	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	145	GLN	4.2
1	D	182	VAL	4.0
1	B	236	ASN	4.0
1	B	334	ALA	3.9
1	B	238	ALA	3.9
1	D	331	ASP	3.9
1	D	328	ASN	3.9
1	B	280	GLY	3.8
1	B	279	SER	3.7
1	D	387	ALA	3.6
1	B	281	ALA	3.6
1	C	356	VAL	3.6
1	B	239	ILE	3.5
1	A	12	MET	3.5
1	B	309	VAL	3.4
1	B	350	GLY	3.4
1	C	317	LEU	3.4
1	A	266	SER	3.3
1	D	41	PRO	3.3
1	D	189	ASP	3.3
1	A	265	ALA	3.2
1	D	236	ASN	3.2
1	A	239	ILE	3.2
1	C	342	LEU	3.1
1	B	226	LYS	3.1
1	D	142	VAL	3.1
1	D	213	LEU	3.1
1	D	391	VAL	3.1
1	A	361	HIS	3.0
1	C	89	VAL	2.9
1	B	395	ILE	2.9
1	C	226	LYS	2.9
1	D	82	ALA	2.9
1	D	265	ALA	2.9
1	B	276	ILE	2.8
1	C	212	VAL	2.8
1	C	213	LEU	2.8
1	A	14	ARG	2.8
1	A	13	LYS	2.8
1	C	214	VAL	2.7
1	B	196	GLU	2.7
1	C	354	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	333	SER	2.7
1	B	348	ILE	2.7
1	D	180	ALA	2.7
1	A	360	LYS	2.7
1	A	291	ASP	2.7
1	D	266	SER	2.7
1	A	144	ALA	2.6
1	D	339	ASP	2.6
1	A	267	GLU	2.6
1	D	285	PHE	2.6
1	B	42	LYS	2.6
1	B	215	ASP	2.6
1	C	217	GLU	2.6
1	A	362	PRO	2.6
1	B	75	ALA	2.6
1	D	13	LYS	2.5
1	D	332	LEU	2.5
1	B	337	LEU	2.5
1	D	507	GLU	2.5
1	A	213	LEU	2.5
1	C	361	HIS	2.5
1	A	391	VAL	2.5
1	C	41	PRO	2.4
1	A	290	ILE	2.4
1	D	78	LEU	2.4
1	D	178	VAL	2.4
1	C	195	ILE	2.4
1	D	321	THR	2.4
1	B	381	ALA	2.4
1	D	340	ALA	2.3
1	D	388	VAL	2.3
1	D	235	LEU	2.3
1	B	325	VAL	2.3
1	D	227	VAL	2.3
1	C	285	PHE	2.3
1	B	213	LEU	2.3
1	B	302	GLY	2.3
1	A	208	LEU	2.3
1	D	264	THR	2.3
1	D	12	MET	2.2
1	A	41	PRO	2.2
1	D	70	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	395	ILE	2.2
1	D	384	VAL	2.2
1	B	351	ASP	2.2
1	A	381	ALA	2.2
1	D	517	ALA	2.2
1	B	343	VAL	2.2
1	A	15	TYR	2.1
1	D	184	ASP	2.1
1	D	465	SER	2.1
1	D	198	LYS	2.1
1	D	392	GLY	2.1
1	B	197	LYS	2.1
1	D	232	ILE	2.1
1	D	179	SER	2.1
1	D	14	ARG	2.1
1	A	42	LYS	2.1
1	B	361	HIS	2.1
1	A	172	GLU	2.1
1	A	217	GLU	2.1
1	C	42	LYS	2.0
1	A	264	THR	2.0
1	C	232	ILE	2.0
1	D	42	LYS	2.0
1	A	368	LEU	2.0
1	B	188	VAL	2.0
1	C	197	LYS	2.0
1	D	208	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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	AGS	B	544	31/31	0.93	0.27	-0.40	255,382,549,549	0
2	AGS	C	544	31/31	0.83	0.27	-0.54	209,414,549,549	0
2	AGS	D	544	31/31	0.87	0.28	-0.54	209,409,549,549	0
2	AGS	A	544	31/31	0.90	0.31	-0.71	260,437,549,549	0

6.5 Other polymers [i](#)

There are no such residues in this entry.