



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:41 PM UTC

PDB ID : 3LDB / pdb_00003ldb
Title : Structure of JMJD6 complexd with ALPHA-KETOGLUTARATE and Fab Fragment.
Authors : Hong, X.; Zang, J.; White, J.; Kappler, J.W.; Wang, C.; Zhang, G.
Deposited on : 2010-01-12
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

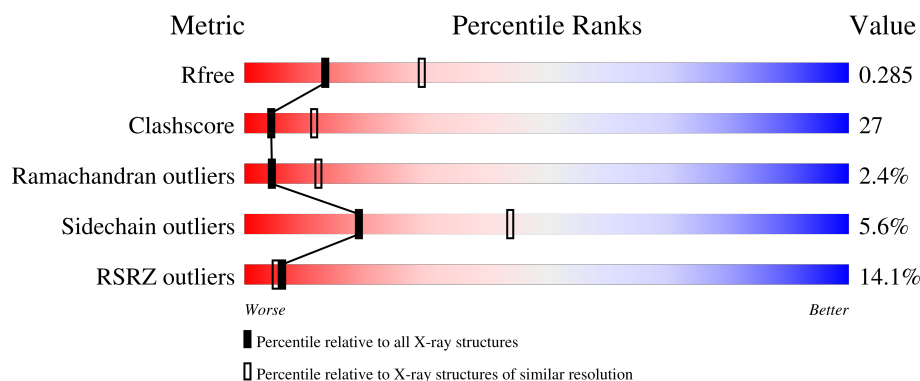
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

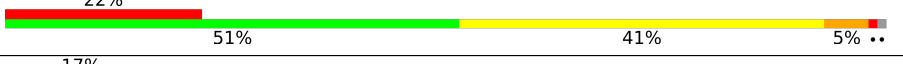
The reported resolution of this entry is 2.70 Å.

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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	334	
2	B	220	
3	C	221	

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
4	GOL	A	336	-	-	X	-
4	GOL	A	337	-	-	X	-
5	SO4	C	223	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6210 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 Bifunctional arginine demethylase and lysyl-hydroxylase JMJD6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2788	1788	492	501	7			

- Molecule 2 is a protein called antibody Fab fragment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	0	0
			1666	1048	275	336	7			

- Molecule 3 is a protein called antibody Fab fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	210	Total	C	N	O	S	0	0	0
			1618	1029	265	318	6			

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



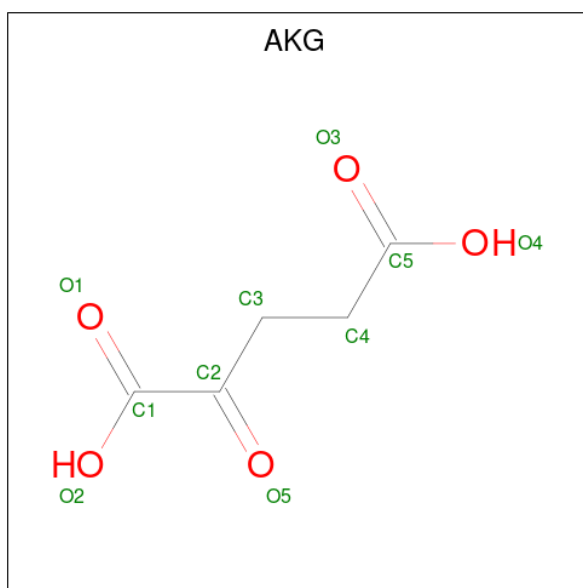
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0
5	A	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		
5	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: C₅H₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			10	5	5		

- Molecule 7 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Fe	0	0
			1	1		

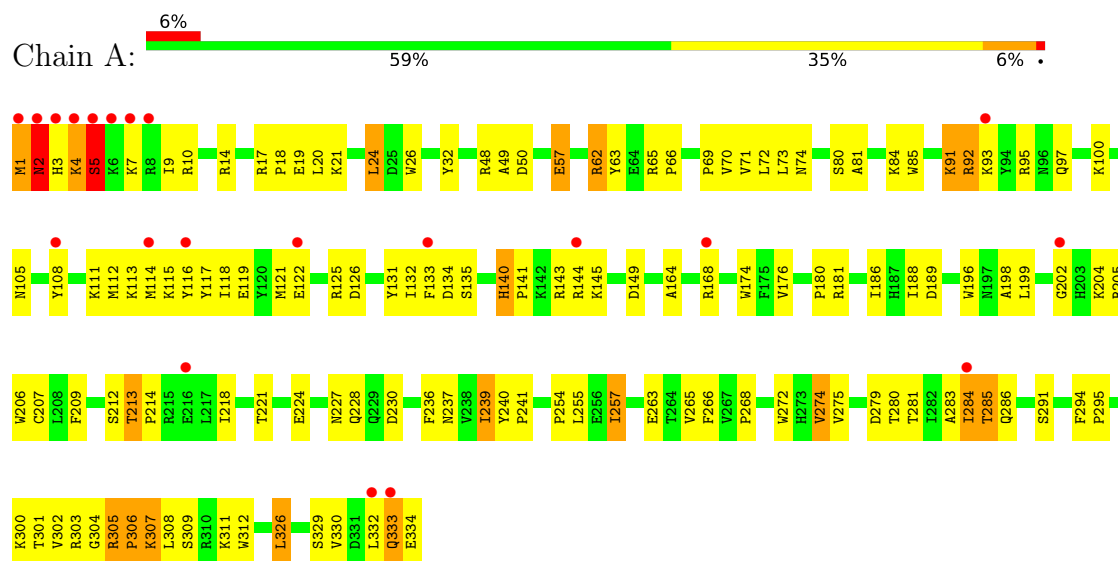
- Molecule 8 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	2	Total	Hg	0	0
			2	2		

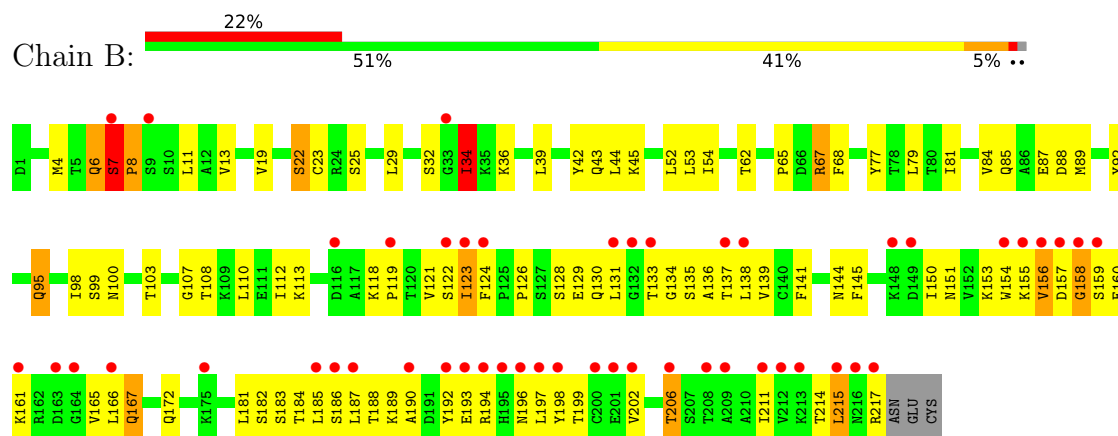
3 Residue-property plots

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

- Molecule 1: Bifunctional arginine demethylase and lysyl-hydroxylase JMJD6

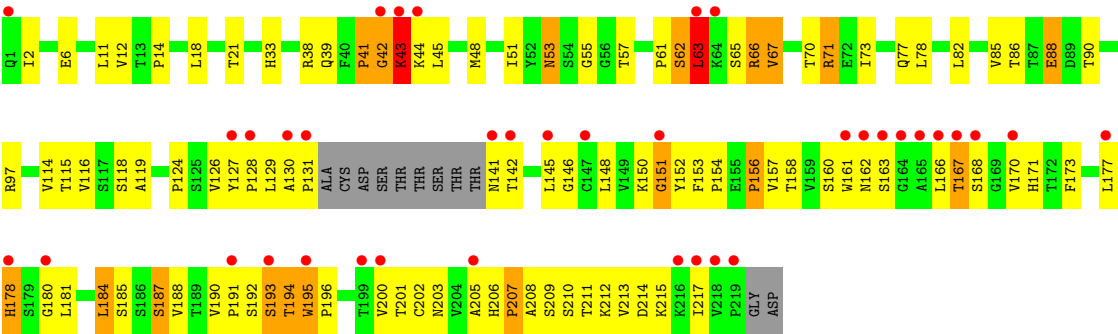


- Molecule 2: antibody Fab fragment light chain



- Molecule 3: antibody Fab fragment heavy chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	138.38Å 138.38Å 183.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.28 – 2.70 47.28 – 2.70	Depositor EDS
% Data completeness (in resolution range)	81.7 (47.28-2.70) 81.7 (47.28-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.250 , 0.285 0.249 , 0.285	Depositor DCC
R_{free} test set	2024 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	63.1	Xtriage
Anisotropy	0.437	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6210	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: FE, HG, GOL, AKG, SO4

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	0.55	2/2873 (0.1%)	1.07	20/3896 (0.5%)
2	B	0.50	1/1699 (0.1%)	1.07	11/2304 (0.5%)
3	C	0.54	0/1664	1.11	10/2282 (0.4%)
All	All	0.53	3/6236 (0.0%)	1.08	41/8482 (0.5%)

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
2	B	0	3
All	All	0	5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5	SER	CA-C	6.59	1.61	1.52
2	B	123	ILE	CA-C	5.14	1.58	1.52
1	A	5	SER	CA-CB	5.08	1.62	1.53

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	42	GLY	N-CA-C	-20.76	86.44	111.35
2	B	7	SER	N-CA-C	11.35	127.60	112.17
2	B	7	SER	CB-CA-C	-10.34	97.34	113.57
2	B	144	ASN	N-CA-C	10.21	132.54	110.80
1	A	2	ASN	N-CA-C	9.54	131.11	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	HIS	CA-C-N	9.30	131.47	119.84
1	A	140	HIS	C-N-CA	9.30	131.47	119.84
2	B	7	SER	CA-C-N	8.86	130.92	119.84
2	B	7	SER	C-N-CA	8.86	130.92	119.84
1	A	239	ILE	N-CA-C	8.77	120.55	111.00
3	C	178	HIS	N-CA-C	7.67	127.13	110.80
1	A	2	ASN	CB-CA-C	-7.24	96.01	110.42
2	B	34	ILE	N-CA-C	-7.14	106.53	113.53
2	B	67	ARG	N-CA-C	-7.01	103.99	112.54
1	A	305	ARG	CA-C-N	6.75	128.27	119.84
1	A	305	ARG	C-N-CA	6.75	128.27	119.84
1	A	312	TRP	N-CA-C	-6.69	103.91	111.07
1	A	24	LEU	N-CA-C	-6.64	105.30	113.41
1	A	228	GLN	N-CA-C	-6.46	103.83	112.94
1	A	21	LYS	N-CA-C	6.43	118.16	111.03
3	C	67	VAL	N-CA-C	6.39	117.98	108.46
3	C	41	PRO	CA-C-N	-6.06	112.57	121.72
3	C	41	PRO	C-N-CA	-6.06	112.57	121.72
3	C	43	LYS	N-CA-C	-5.78	98.49	110.80
2	B	121	VAL	N-CA-C	5.74	116.98	109.58
1	A	257	ILE	N-CA-C	5.60	116.19	108.12
1	A	189	ASP	CA-C-N	5.58	125.52	119.78
1	A	189	ASP	C-N-CA	5.58	125.52	119.78
3	C	55	GLY	N-CA-C	-5.53	107.41	114.37
1	A	213	THR	CA-C-N	5.49	125.66	119.90
1	A	213	THR	C-N-CA	5.49	125.66	119.90
2	B	99	SER	N-CA-C	5.47	118.32	108.48
1	A	63	TYR	N-CA-C	5.43	119.39	112.12
2	B	103	THR	N-CA-C	5.21	117.85	110.50
1	A	230	ASP	N-CA-C	5.21	118.76	112.93
3	C	178	HIS	CB-CA-C	-5.19	100.10	110.42
1	A	255	LEU	N-CA-C	-5.15	101.31	109.76
1	A	164	ALA	N-CA-C	-5.09	107.04	114.12
2	B	22	SER	N-CA-C	5.07	118.02	109.95
3	C	118	SER	N-CA-C	-5.03	107.27	113.41
3	C	187	SER	N-CA-C	5.01	115.59	107.23

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	MET	Peptide

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Mol	Chain	Res	Type	Group
1	A	2	ASN	Peptide
2	B	156	VAL	Peptide
2	B	6	GLN	Peptide
2	B	7	SER	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	2788	0	2739	124	0
2	B	1666	0	1644	114	0
3	C	1618	0	1568	102	0
4	A	24	0	28	10	0
4	B	6	0	7	0	0
5	A	65	0	0	2	0
5	B	15	0	0	0	0
5	C	15	0	0	0	0
6	A	10	0	4	0	0
7	A	1	0	0	0	0
8	A	2	0	0	0	0
All	All	6210	0	5990	325	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 27.

All (325) 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)
2:B:7:SER:HB2	2:B:8:PRO:CD	1.64	1.27
2:B:167:GLN:HB3	2:B:183:SER:HA	1.38	1.06
2:B:7:SER:HB2	2:B:8:PRO:HD2	1.43	1.00
2:B:7:SER:HB2	2:B:8:PRO:HD3	1.42	0.98
2:B:7:SER:CB	2:B:8:PRO:CD	2.42	0.98
2:B:7:SER:CB	2:B:8:PRO:HD2	1.98	0.94
1:A:141:PRO:HA	1:A:144:ARG:HH11	1.33	0.93
2:B:137:THR:HG22	2:B:186:SER:HA	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:VAL:HB	2:B:185:LEU:HD13	1.56	0.88
3:C:124:PRO:HB3	3:C:152:TYR:HB3	1.56	0.87
1:A:57:GLU:OE1	3:C:33:HIS:HE1	1.58	0.85
2:B:126:PRO:HD3	2:B:138:LEU:HG	1.59	0.84
3:C:63:LEU:HD12	3:C:63:LEU:O	1.78	0.83
2:B:217:ARG:HG2	2:B:217:ARG:HH11	1.44	0.83
3:C:53:ASN:HD22	3:C:53:ASN:H	1.23	0.82
1:A:206:TRP:HB2	1:A:257:ILE:HB	1.62	0.81
1:A:329:SER:O	1:A:333:GLN:HB2	1.79	0.81
2:B:118:LYS:HG2	2:B:206:THR:HG21	1.62	0.81
1:A:141:PRO:HA	1:A:144:ARG:NH1	1.95	0.80
2:B:118:LYS:HG2	2:B:206:THR:CG2	2.12	0.80
3:C:166:LEU:HD13	3:C:188:VAL:HG21	1.64	0.79
2:B:39:LEU:HD22	2:B:77:TYR:CG	2.19	0.78
2:B:181:LEU:HD23	2:B:182:SER:N	1.99	0.78
1:A:168:ARG:HD2	1:A:311:LYS:CD	2.13	0.78
2:B:198:TYR:O	2:B:214:THR:HG23	1.85	0.77
2:B:151:ASN:HD21	2:B:153:LYS:HE3	1.49	0.77
1:A:199:LEU:HD13	1:A:204:LYS:HE2	1.67	0.76
2:B:137:THR:CG2	2:B:186:SER:HA	2.15	0.75
2:B:156:VAL:HG23	2:B:160:GLU:HB2	1.65	0.75
1:A:48:ARG:HD3	1:A:71:VAL:HB	1.67	0.75
1:A:332:LEU:C	1:A:334:GLU:H	1.94	0.75
1:A:112:MET:HE2	1:A:117:TYR:HA	1.68	0.74
1:A:284:ILE:HD13	1:A:285:THR:N	2.03	0.73
3:C:85:VAL:HG12	3:C:116:VAL:HG11	1.71	0.72
1:A:80:SER:OG	1:A:149:ASP:HA	1.90	0.72
2:B:167:GLN:HB3	2:B:183:SER:CA	2.18	0.72
3:C:53:ASN:HD22	3:C:53:ASN:N	1.88	0.71
2:B:160:GLU:HG2	2:B:161:LYS:N	2.06	0.71
1:A:18:PRO:HG2	1:A:105:ASN:ND2	2.06	0.71
2:B:7:SER:CB	2:B:22:SER:H	2.03	0.71
3:C:142:THR:HA	3:C:192:SER:HB2	1.71	0.70
2:B:137:THR:HG21	3:C:150:LYS:HE3	1.74	0.70
3:C:214:ASP:O	3:C:215:LYS:HG2	1.92	0.69
2:B:155:LYS:HB2	2:B:199:THR:OG1	1.92	0.69
3:C:145:LEU:HD22	3:C:200:VAL:HG11	1.73	0.68
2:B:165:VAL:O	2:B:166:LEU:HD12	1.93	0.68
2:B:7:SER:OG	2:B:22:SER:N	2.25	0.68
1:A:221:THR:OG1	1:A:224:GLU:HG3	1.94	0.68
2:B:42:TYR:HE1	2:B:95:GLN:HG2	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:GLU:HG2	2:B:161:LYS:H	1.58	0.68
1:A:1:MET:H2	1:A:2:ASN:HA	1.60	0.66
2:B:199:THR:HG22	2:B:214:THR:OG1	1.95	0.66
2:B:130:GLN:HB2	3:C:127:TYR:CG	2.30	0.66
1:A:326:LEU:O	1:A:329:SER:HB3	1.95	0.66
2:B:7:SER:HB3	2:B:22:SER:HB3	1.77	0.65
2:B:139:VAL:HG21	3:C:129:LEU:HD13	1.79	0.65
1:A:57:GLU:OE1	3:C:33:HIS:CE1	2.46	0.65
1:A:4:LYS:O	1:A:7:LYS:N	2.30	0.65
1:A:209:PHE:CE1	1:A:254:PRO:HB3	2.32	0.64
2:B:67:ARG:NH2	2:B:88:ASP:OD1	2.29	0.64
1:A:18:PRO:HG2	1:A:105:ASN:HD21	1.61	0.64
2:B:124:PHE:CD2	3:C:129:LEU:HB3	2.33	0.64
3:C:167:THR:HG23	3:C:168:SER:H	1.63	0.63
1:A:1:MET:N	1:A:2:ASN:HA	2.11	0.63
3:C:63:LEU:CD1	3:C:67:VAL:HG21	2.27	0.63
3:C:157:VAL:HG23	3:C:184:LEU:HD21	1.80	0.63
2:B:217:ARG:HG2	2:B:217:ARG:NH1	2.14	0.62
1:A:92:ARG:HH11	1:A:92:ARG:HB2	1.63	0.62
3:C:33:HIS:HD2	3:C:53:ASN:H	1.48	0.62
1:A:180:PRO:HB3	1:A:279:ASP:HA	1.82	0.62
3:C:151:GLY:C	3:C:181:LEU:HD23	2.25	0.62
1:A:140:HIS:HB3	5:A:344:SO4:O4	2.00	0.62
1:A:91:LYS:HB2	1:A:118:ILE:HD12	1.82	0.61
3:C:11:LEU:HD22	3:C:154:PRO:HD3	1.83	0.61
3:C:126:VAL:HG21	3:C:213:VAL:HG21	1.82	0.61
1:A:62:ARG:HG3	1:A:62:ARG:HH11	1.64	0.61
2:B:139:VAL:HG12	2:B:184:THR:HG22	1.83	0.61
1:A:7:LYS:HE3	1:A:10:ARG:NH2	2.16	0.60
1:A:280:THR:H	4:A:336:GOL:H11	1.66	0.60
3:C:51:ILE:HA	3:C:57:THR:HG22	1.83	0.60
2:B:124:PHE:HB3	3:C:129:LEU:HD22	1.85	0.59
2:B:165:VAL:C	2:B:166:LEU:HD12	2.26	0.59
2:B:8:PRO:O	2:B:108:THR:HG23	2.03	0.59
3:C:63:LEU:HD12	3:C:67:VAL:HG21	1.84	0.59
2:B:11:LEU:HD12	2:B:11:LEU:C	2.29	0.58
1:A:9:ILE:HD12	4:A:337:GOL:H11	1.86	0.57
3:C:201:THR:HG23	3:C:215:LYS:H	1.70	0.57
1:A:266:PHE:CE2	1:A:268:PRO:HG3	2.39	0.57
3:C:90:THR:HG23	3:C:115:THR:HA	1.86	0.57
3:C:178:HIS:ND1	3:C:178:HIS:C	2.62	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:SER:OG	2:B:8:PRO:HD2	2.05	0.56
1:A:92:ARG:HB2	1:A:92:ARG:NH1	2.20	0.56
3:C:201:THR:HG23	3:C:215:LYS:C	2.30	0.56
2:B:202:VAL:HB	2:B:211:ILE:HG23	1.87	0.56
3:C:53:ASN:H	3:C:53:ASN:ND2	2.01	0.56
1:A:81:ALA:O	1:A:85:TRP:HB2	2.04	0.56
1:A:112:MET:HE3	1:A:116:TYR:CB	2.36	0.56
2:B:126:PRO:CB	2:B:136:ALA:HB1	2.36	0.56
1:A:168:ARG:HD2	1:A:311:LYS:HD2	1.88	0.55
2:B:43:GLN:HB2	2:B:53:LEU:HD11	1.89	0.55
2:B:129:GLU:HG2	3:C:215:LYS:NZ	2.21	0.55
1:A:117:TYR:CE2	1:A:121:MET:HG3	2.42	0.55
1:A:70:VAL:HG22	1:A:71:VAL:N	2.21	0.55
2:B:133:THR:HG22	2:B:134:GLY:N	2.22	0.55
3:C:190:VAL:HB	3:C:191:PRO:HD2	1.89	0.55
1:A:81:ALA:HB1	1:A:85:TRP:CD2	2.42	0.55
1:A:118:ILE:O	1:A:122:GLU:HG3	2.07	0.54
2:B:124:PHE:HB2	2:B:139:VAL:CG2	2.37	0.54
3:C:177:LEU:HD23	3:C:178:HIS:N	2.23	0.54
3:C:191:PRO:HG2	3:C:194:THR:HG22	1.88	0.54
3:C:67:VAL:HG22	3:C:82:LEU:CD1	2.38	0.54
2:B:42:TYR:CE1	2:B:95:GLN:HG2	2.41	0.54
1:A:332:LEU:C	1:A:334:GLU:N	2.64	0.54
1:A:279:ASP:HB2	4:A:336:GOL:H32	1.90	0.54
2:B:67:ARG:HH21	2:B:88:ASP:CG	2.15	0.54
2:B:133:THR:C	2:B:135:SER:H	2.16	0.54
2:B:19:VAL:HG12	2:B:81:ILE:HB	1.91	0.53
3:C:191:PRO:HG2	3:C:194:THR:CG2	2.39	0.53
1:A:168:ARG:HD2	1:A:311:LYS:HD3	1.88	0.53
2:B:7:SER:HG	2:B:22:SER:N	2.07	0.53
3:C:67:VAL:HG22	3:C:82:LEU:HD13	1.91	0.53
1:A:332:LEU:O	1:A:334:GLU:N	2.42	0.53
3:C:184:LEU:HD12	3:C:184:LEU:C	2.34	0.52
2:B:110:LEU:HD23	2:B:110:LEU:C	2.35	0.52
3:C:141:ASN:O	3:C:192:SER:HB2	2.10	0.52
1:A:19:GLU:HG3	1:A:227:ASN:HB2	1.92	0.52
1:A:188:ILE:HD11	1:A:272:TRP:CE2	2.44	0.52
1:A:4:LYS:O	1:A:5:SER:C	2.53	0.52
1:A:84:LYS:NZ	1:A:93:LYS:NZ	2.58	0.52
1:A:302:VAL:HG23	1:A:303:ARG:N	2.25	0.52
1:A:1:MET:HG3	4:A:337:GOL:O3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:LYS:HB2	1:A:307:LYS:NZ	2.25	0.51
3:C:42:GLY:O	3:C:43:LYS:HG2	2.10	0.51
1:A:135:SER:HB3	1:A:174:TRP:CD1	2.45	0.51
3:C:38:ARG:HB3	3:C:48:MET:HE1	1.91	0.51
3:C:53:ASN:N	3:C:53:ASN:ND2	2.57	0.51
3:C:63:LEU:HD13	3:C:67:VAL:HG21	1.93	0.51
1:A:1:MET:HG3	4:A:337:GOL:C2	2.41	0.51
1:A:117:TYR:CE2	1:A:121:MET:HE2	2.45	0.51
1:A:26:TRP:HB3	1:A:126:ASP:OD1	2.11	0.51
1:A:196:TRP:HA	1:A:265:VAL:O	2.10	0.51
2:B:131:LEU:HD11	2:B:189:LYS:HG3	1.92	0.51
2:B:133:THR:HG22	2:B:134:GLY:H	1.74	0.51
1:A:168:ARG:CD	1:A:311:LYS:HD2	2.40	0.51
1:A:117:TYR:OH	1:A:131:TYR:HA	2.10	0.50
2:B:32:SER:C	2:B:34:ILE:H	2.20	0.50
2:B:45:LYS:HE2	2:B:87:GLU:O	2.11	0.50
3:C:86:THR:O	3:C:116:VAL:HG11	2.12	0.50
3:C:160:SER:OG	3:C:203:ASN:HB2	2.12	0.50
3:C:195:TRP:CD1	3:C:195:TRP:C	2.88	0.50
1:A:284:ILE:HD13	1:A:284:ILE:C	2.36	0.49
2:B:6:GLN:OE1	2:B:107:GLY:N	2.43	0.49
1:A:10:ARG:HH11	1:A:14:ARG:HH21	1.60	0.49
3:C:160:SER:O	3:C:203:ASN:N	2.37	0.49
2:B:124:PHE:HB2	2:B:139:VAL:HG22	1.94	0.49
3:C:85:VAL:HG12	3:C:86:THR:N	2.28	0.49
1:A:112:MET:HE2	1:A:117:TYR:CA	2.39	0.49
3:C:201:THR:CG2	3:C:215:LYS:H	2.24	0.49
1:A:300:LYS:HE3	5:A:347:SO4:O4	2.12	0.49
3:C:51:ILE:HD11	3:C:71:ARG:HD2	1.93	0.49
3:C:145:LEU:N	3:C:145:LEU:HD12	2.27	0.49
1:A:133:PHE:CD1	1:A:133:PHE:O	2.66	0.49
1:A:134:ASP:OD1	1:A:143:ARG:NH1	2.44	0.49
2:B:193:GLU:CB	2:B:217:ARG:HH21	2.25	0.49
2:B:139:VAL:HG21	3:C:129:LEU:CD1	2.42	0.49
3:C:51:ILE:HG23	3:C:51:ILE:O	2.13	0.49
3:C:39:GLN:HA	3:C:44:LYS:O	2.13	0.48
2:B:196:ASN:O	2:B:217:ARG:HB2	2.13	0.48
3:C:158:THR:OG1	3:C:205:ALA:HB3	2.13	0.48
1:A:280:THR:H	4:A:336:GOL:C1	2.26	0.48
2:B:6:GLN:NE2	2:B:107:GLY:HA2	2.28	0.48
2:B:126:PRO:CD	2:B:138:LEU:HG	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:39:GLN:HB2	3:C:45:LEU:CD2	2.44	0.48
1:A:69:PRO:HB3	1:A:268:PRO:HD3	1.95	0.48
2:B:129:GLU:HG2	3:C:215:LYS:HZ1	1.79	0.48
1:A:205:ARG:CZ	1:A:236:PHE:CE1	2.97	0.47
2:B:154:TRP:HD1	2:B:165:VAL:HG21	1.78	0.47
2:B:141:PHE:CE2	3:C:187:SER:HB2	2.49	0.47
3:C:128:PRO:CG	3:C:215:LYS:HD2	2.44	0.47
2:B:34:ILE:HG23	2:B:36:LYS:HG2	1.97	0.47
1:A:291:SER:HB3	2:B:32:SER:OG	2.13	0.47
2:B:84:VAL:HG12	2:B:85:GLN:N	2.29	0.47
3:C:2:ILE:CD1	3:C:97:ARG:HD3	2.45	0.47
3:C:145:LEU:HD23	3:C:217:ILE:HG21	1.95	0.47
1:A:279:ASP:O	1:A:281:THR:HG23	2.15	0.47
1:A:3:HIS:CD2	1:A:3:HIS:O	2.67	0.47
2:B:11:LEU:HD11	2:B:19:VAL:HG21	1.97	0.47
2:B:137:THR:HG22	2:B:187:LEU:H	1.80	0.47
2:B:138:LEU:N	2:B:138:LEU:HD12	2.30	0.47
3:C:162:ASN:N	3:C:201:THR:O	2.30	0.47
1:A:186:ILE:CA	1:A:274:VAL:HG13	2.46	0.46
3:C:38:ARG:NH2	3:C:63:LEU:HD22	2.30	0.46
3:C:85:VAL:CG1	3:C:116:VAL:HG21	2.46	0.46
2:B:155:LYS:HD2	2:B:158:GLY:O	2.16	0.46
1:A:279:ASP:HB2	4:A:336:GOL:H12	1.96	0.46
2:B:167:GLN:HE21	2:B:181:LEU:HD11	1.80	0.46
2:B:196:ASN:ND2	2:B:197:LEU:CD1	2.79	0.46
2:B:217:ARG:NH1	2:B:217:ARG:CG	2.79	0.46
3:C:148:LEU:HD13	3:C:148:LEU:C	2.41	0.46
2:B:128:SER:O	2:B:129:GLU:C	2.57	0.46
1:A:301:THR:HG22	1:A:309:SER:HB3	1.97	0.46
2:B:13:VAL:HG11	2:B:19:VAL:HB	1.98	0.46
3:C:126:VAL:HG21	3:C:213:VAL:CG2	2.46	0.46
1:A:1:MET:HB2	1:A:5:SER:OG	2.15	0.46
1:A:280:THR:OG1	4:A:336:GOL:H11	2.15	0.46
2:B:34:ILE:HG23	2:B:36:LYS:CG	2.46	0.46
2:B:42:TYR:HE1	2:B:95:GLN:CG	2.27	0.46
1:A:140:HIS:HA	1:A:141:PRO:HD3	1.82	0.45
1:A:100:LYS:HE2	1:A:133:PHE:CE1	2.51	0.45
2:B:181:LEU:HD23	2:B:181:LEU:C	2.40	0.45
3:C:66:ARG:O	3:C:82:LEU:HA	2.16	0.45
3:C:177:LEU:HD23	3:C:177:LEU:C	2.40	0.45
1:A:132:ILE:O	1:A:176:VAL:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:LYS:HB2	1:A:311:LYS:HE2	1.86	0.45
2:B:124:PHE:CB	3:C:129:LEU:HD22	2.46	0.45
2:B:7:SER:HB3	2:B:22:SER:CB	2.43	0.45
3:C:85:VAL:CG1	3:C:86:THR:N	2.78	0.45
3:C:195:TRP:HB3	3:C:196:PRO:CD	2.46	0.45
1:A:330:VAL:HA	1:A:333:GLN:CB	2.46	0.45
1:A:91:LYS:O	1:A:95:ARG:HB2	2.17	0.45
1:A:180:PRO:O	1:A:181:ARG:HB2	2.16	0.45
2:B:4:MET:HE3	2:B:23:CYS:SG	2.56	0.45
3:C:85:VAL:HG12	3:C:116:VAL:CG1	2.42	0.45
2:B:89:MET:HE3	2:B:172:GLN:HB3	1.98	0.45
2:B:196:ASN:ND2	2:B:197:LEU:HD12	2.31	0.45
1:A:143:ARG:O	1:A:144:ARG:C	2.60	0.45
1:A:10:ARG:HH11	1:A:10:ARG:HG2	1.81	0.44
3:C:173:PHE:N	3:C:173:PHE:CD2	2.85	0.44
1:A:49:ALA:HB3	1:A:72:LEU:HD23	1.99	0.44
2:B:155:LYS:HB3	2:B:157:ASP:O	2.18	0.44
3:C:128:PRO:HG3	3:C:215:LYS:HD2	1.98	0.44
2:B:6:GLN:HE22	2:B:107:GLY:HA2	1.82	0.44
2:B:119:PRO:HG3	2:B:145:PHE:CB	2.47	0.44
2:B:192:TYR:C	2:B:194:ARG:H	2.26	0.44
1:A:168:ARG:CD	1:A:311:LYS:CD	2.90	0.44
1:A:199:LEU:HD21	1:A:202:GLY:O	2.17	0.44
1:A:294:PHE:HB3	1:A:295:PRO:HD3	1.99	0.44
2:B:167:GLN:NE2	2:B:181:LEU:HD11	2.32	0.44
3:C:191:PRO:O	3:C:192:SER:C	2.60	0.44
1:A:213:THR:HA	1:A:214:PRO:HD3	1.79	0.44
2:B:190:ALA:O	2:B:194:ARG:HB2	2.18	0.44
1:A:62:ARG:HH11	1:A:62:ARG:CG	2.29	0.43
2:B:39:LEU:HD22	2:B:77:TYR:CD1	2.53	0.43
2:B:92:TYR:O	2:B:107:GLY:HA2	2.18	0.43
2:B:122:SER:HB3	2:B:124:PHE:HE1	1.83	0.43
1:A:91:LYS:HB2	1:A:118:ILE:CD1	2.48	0.43
3:C:86:THR:OG1	3:C:88:GLU:HG2	2.18	0.43
1:A:115:LYS:O	1:A:119:GLU:HG3	2.19	0.43
2:B:150:ILE:HG12	2:B:151:ASN:N	2.34	0.43
3:C:63:LEU:O	3:C:63:LEU:CD1	2.58	0.43
1:A:32:TYR:CE2	1:A:125:ARG:NH1	2.86	0.43
1:A:330:VAL:HA	1:A:333:GLN:HB3	2.01	0.43
1:A:9:ILE:HD12	4:A:337:GOL:C1	2.49	0.43
1:A:286:GLN:HE21	1:A:286:GLN:HB3	1.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:141:ASN:C	3:C:141:ASN:ND2	2.75	0.43
1:A:108:TYR:N	1:A:108:TYR:CD2	2.85	0.43
2:B:160:GLU:CG	2:B:161:LYS:N	2.80	0.43
1:A:2:ASN:N	1:A:5:SER:OG	2.52	0.43
3:C:130:ALA:HB1	3:C:131:PRO:CD	2.49	0.43
2:B:100:ASN:OD1	3:C:61:PRO:HD3	2.19	0.43
3:C:206:HIS:HD2	3:C:209:SER:OG	2.02	0.43
1:A:114:MET:HE1	1:A:132:ILE:CD1	2.49	0.42
1:A:112:MET:CE	1:A:117:TYR:HA	2.44	0.42
3:C:161:TRP:O	3:C:163:SER:O	2.36	0.42
2:B:196:ASN:HD22	2:B:197:LEU:CD1	2.32	0.42
3:C:206:HIS:HB3	3:C:211:THR:HB	2.00	0.42
1:A:206:TRP:CD2	1:A:275:VAL:HG22	2.54	0.42
1:A:240:TYR:N	1:A:241:PRO:CD	2.81	0.42
3:C:180:GLY:C	3:C:181:LEU:HD12	2.44	0.42
1:A:97:GLN:O	1:A:113:LYS:HA	2.19	0.42
1:A:112:MET:HE3	1:A:116:TYR:HB2	2.02	0.42
3:C:18:LEU:HD13	3:C:114:VAL:HG11	2.01	0.42
3:C:161:TRP:HA	3:C:202:CYS:HA	2.02	0.42
1:A:305:ARG:O	1:A:308:LEU:HB3	2.20	0.42
3:C:6:GLU:HA	3:C:21:THR:O	2.20	0.42
3:C:78:LEU:N	3:C:78:LEU:HD22	2.34	0.42
3:C:126:VAL:CG2	3:C:213:VAL:HG21	2.49	0.42
2:B:65:PRO:HG2	2:B:68:PHE:CE2	2.55	0.41
2:B:92:TYR:CD1	2:B:92:TYR:N	2.88	0.41
1:A:73:LEU:CD2	1:A:263:GLU:HG2	2.50	0.41
1:A:117:TYR:CD2	1:A:121:MET:HE2	2.55	0.41
1:A:112:MET:HE3	1:A:117:TYR:N	2.36	0.41
1:A:218:ILE:HA	1:A:239:ILE:HD13	2.02	0.41
2:B:122:SER:HB3	2:B:124:PHE:CE1	2.56	0.41
3:C:141:ASN:C	3:C:141:ASN:HD22	2.27	0.41
1:A:17:ARG:HG3	1:A:17:ARG:HH11	1.86	0.41
2:B:119:PRO:HG3	2:B:145:PHE:HB3	2.03	0.41
2:B:182:SER:HB2	3:C:173:PHE:CD1	2.54	0.41
3:C:170:VAL:O	3:C:171:HIS:HD2	2.03	0.41
1:A:19:GLU:HG2	1:A:20:LEU:N	2.34	0.41
1:A:65:ARG:HB3	1:A:66:PRO:HD3	2.01	0.41
1:A:91:LYS:NZ	1:A:91:LYS:HB3	2.36	0.41
1:A:112:MET:HE3	1:A:116:TYR:HB3	2.02	0.41
3:C:129:LEU:HB2	3:C:146:GLY:O	2.20	0.41
1:A:50:ASP:OD1	1:A:74:ASN:ND2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:62:SER:OG	3:C:63:LEU:N	2.52	0.41
1:A:1:MET:HG3	4:A:337:GOL:O2	2.21	0.41
1:A:305:ARG:N	1:A:306:PRO:HD3	2.36	0.41
3:C:33:HIS:CD2	3:C:53:ASN:H	2.33	0.41
3:C:184:LEU:C	3:C:184:LEU:CD1	2.94	0.41
1:A:100:LYS:HA	1:A:111:LYS:HG2	2.02	0.41
1:A:143:ARG:C	1:A:145:LYS:N	2.77	0.41
1:A:186:ILE:HA	1:A:274:VAL:HG13	2.03	0.41
1:A:198:ALA:O	1:A:283:ALA:HB1	2.20	0.41
2:B:19:VAL:CG1	2:B:81:ILE:HB	2.50	0.41
2:B:98:ILE:O	2:B:98:ILE:HG13	2.21	0.41
3:C:39:GLN:HA	3:C:45:LEU:HD23	2.02	0.41
3:C:207:PRO:O	3:C:208:ALA:C	2.64	0.41
1:A:279:ASP:OD1	1:A:279:ASP:C	2.63	0.41
2:B:112:ILE:HG22	2:B:113:LYS:N	2.33	0.41
2:B:165:VAL:O	2:B:165:VAL:HG13	2.21	0.41
3:C:12:VAL:O	3:C:116:VAL:HA	2.20	0.41
3:C:193:SER:O	3:C:195:TRP:N	2.51	0.41
1:A:304:GLY:O	1:A:305:ARG:HG2	2.22	0.40
2:B:188:THR:HG22	2:B:190:ALA:H	1.86	0.40
3:C:153:PHE:CD1	3:C:153:PHE:C	2.99	0.40
1:A:140:HIS:CD2	1:A:143:ARG:NH2	2.89	0.40
2:B:123:ILE:HG23	2:B:215:LEU:HD23	2.03	0.40
1:A:112:MET:CE	1:A:117:TYR:N	2.84	0.40
2:B:25:SER:OG	2:B:29:LEU:HD11	2.22	0.40
2:B:126:PRO:HB3	2:B:136:ALA:HB1	2.03	0.40
1:A:1:MET:N	1:A:1:MET:SD	2.91	0.40
2:B:54:ILE:HD12	2:B:79:LEU:CD1	2.51	0.40
3:C:151:GLY:CA	3:C:181:LEU:HD23	2.51	0.40
2:B:11:LEU:HD12	2:B:11:LEU:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	332/334 (99%)	305 (92%)	24 (7%)	3 (1%)	14	35
2	B	215/220 (98%)	181 (84%)	31 (14%)	3 (1%)	9	23
3	C	206/221 (93%)	175 (85%)	19 (9%)	12 (6%)	1	2
All	All	753/775 (97%)	661 (88%)	74 (10%)	18 (2%)	4	12

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	206	THR
3	C	62	SER
3	C	193	SER
3	C	194	THR
1	A	333	GLN
3	C	43	LYS
3	C	151	GLY
3	C	119	ALA
3	C	167	THR
3	C	210	SER
3	C	195	TRP
1	A	5	SER
1	A	306	PRO
2	B	8	PRO
2	B	158	GLY
3	C	63	LEU
3	C	14	PRO
3	C	156	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	301/301 (100%)	287 (95%)	14 (5%)	23	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	190/193 (98%)	181 (95%)	9 (5%)	23	51
3	C	187/196 (95%)	172 (92%)	15 (8%)	11	28
All	All	678/690 (98%)	640 (94%)	38 (6%)	19	44

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	24	LEU
1	A	57	GLU
1	A	62	ARG
1	A	91	LYS
1	A	92	ARG
1	A	207	CYS
1	A	212	SER
1	A	237	ASN
1	A	274	VAL
1	A	284	ILE
1	A	285	THR
1	A	307	LYS
1	A	326	LEU
2	B	7	SER
2	B	34	ILE
2	B	44	LEU
2	B	52	LEU
2	B	62	THR
2	B	95	GLN
2	B	159	SER
2	B	167	GLN
2	B	215	LEU
3	C	41	PRO
3	C	53	ASN
3	C	63	LEU
3	C	65	SER
3	C	66	ARG
3	C	70	THR
3	C	71	ARG
3	C	73	ILE
3	C	77	GLN
3	C	88	GLU
3	C	156	PRO

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Mol	Chain	Res	Type
3	C	184	LEU
3	C	185	SER
3	C	207	PRO
3	C	212	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	29	HIS
1	A	30	ASN
1	A	97	GLN
1	A	105	ASN
1	A	140	HIS
1	A	197	ASN
1	A	237	ASN
1	A	286	GLN
1	A	333	GLN
2	B	27	GLN
2	B	95	GLN
2	B	130	GLN
2	B	143	ASN
2	B	151	ASN
2	B	167	GLN
2	B	196	ASN
3	C	33	HIS
3	C	53	ASN
3	C	81	GLN
3	C	141	ASN
3	C	171	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 3 are monoatomic - leaving 25 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	338	-	5,5,5	2.19	1 (20%)	5,5,5	0.36	0
6	AKG	A	600	-	9,9,9	1.40	2 (22%)	11,11,11	1.45	2 (18%)
5	SO4	A	339	-	4,4,4	0.37	0	6,6,6	0.17	0
5	SO4	A	343	-	4,4,4	0.37	0	6,6,6	0.07	0
5	SO4	A	341	-	4,4,4	0.37	0	6,6,6	0.13	0
4	GOL	A	337	-	5,5,5	2.15	1 (20%)	5,5,5	0.35	0
5	SO4	C	223	-	4,4,4	0.35	0	6,6,6	0.08	0
5	SO4	C	224	-	4,4,4	0.38	0	6,6,6	0.10	0
5	SO4	A	349	-	4,4,4	0.36	0	6,6,6	0.09	0
5	SO4	A	342	-	4,4,4	0.40	0	6,6,6	0.06	0
5	SO4	A	344	-	4,4,4	0.37	0	6,6,6	0.08	0
5	SO4	B	223	-	4,4,4	0.41	0	6,6,6	0.11	0
5	SO4	B	224	-	4,4,4	0.34	0	6,6,6	0.19	0
5	SO4	A	351	-	4,4,4	0.36	0	6,6,6	0.09	0
5	SO4	A	347	-	4,4,4	0.36	0	6,6,6	0.09	0
5	SO4	A	345	-	4,4,4	0.36	0	6,6,6	0.14	0
4	GOL	B	221	-	5,5,5	2.17	1 (20%)	5,5,5	0.28	0
5	SO4	C	222	-	4,4,4	0.39	0	6,6,6	0.12	0
5	SO4	A	346	-	4,4,4	0.38	0	6,6,6	0.06	0
5	SO4	A	348	-	4,4,4	0.39	0	6,6,6	0.06	0
5	SO4	B	222	-	4,4,4	0.38	0	6,6,6	0.10	0
5	SO4	A	350	-	4,4,4	0.36	0	6,6,6	0.21	0
4	GOL	A	335	-	5,5,5	2.18	1 (20%)	5,5,5	0.40	0
4	GOL	A	336	-	5,5,5	2.28	1 (20%)	5,5,5	0.46	0
5	SO4	A	340	-	4,4,4	0.37	0	6,6,6	0.12	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
4	GOL	A	338	-	-	0/4/4/4	-
4	GOL	A	337	-	-	0/4/4/4	-
6	AKG	A	600	-	-	0/9/9/9	-
4	GOL	B	221	-	-	0/4/4/4	-
4	GOL	A	335	-	-	0/4/4/4	-
4	GOL	A	336	-	-	0/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	336	GOL	O1-C1	-5.00	1.21	1.42
4	A	338	GOL	O1-C1	-4.80	1.22	1.42
4	B	221	GOL	O1-C1	-4.80	1.22	1.42
4	A	337	GOL	O1-C1	-4.78	1.22	1.42
4	A	335	GOL	O1-C1	-4.77	1.22	1.42
6	A	600	AKG	C3-C2	2.98	1.54	1.51
6	A	600	AKG	O2-C1	2.26	1.36	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	600	AKG	C3-C2-C1	2.50	120.11	115.86
6	A	600	AKG	O2-C1-C2	2.31	120.00	113.59

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	337	GOL	5	0
5	A	344	SO4	1	0
5	A	347	SO4	1	0
4	A	336	GOL	5	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	334/334 (100%)	0.64	21 (6%) 26 23	23, 69, 104, 129	3 (0%)
2	B	217/220 (98%)	1.12	49 (22%) 2 2	34, 77, 148, 159	0
3	C	210/221 (95%)	1.01	37 (17%) 4 3	33, 84, 136, 141	0
All	All	761/775 (98%)	0.88	107 (14%) 6 5	23, 74, 141, 159	3 (0%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	PHE	10.8
1	A	2	ASN	10.1
1	A	1	MET	9.6
2	B	215	LEU	8.2
2	B	123	ILE	8.0
3	C	162	ASN	6.2
3	C	219	PRO	6.0
1	A	144	ARG	5.9
1	A	3	HIS	5.8
1	A	5	SER	5.7
2	B	156	VAL	5.5
2	B	209	ALA	5.4
3	C	199	THR	5.3
1	A	6	LYS	5.3
3	C	42	GLY	5.1
1	A	4	LYS	5.0
2	B	7	SER	4.9
3	C	164	GLY	4.9
3	C	43	LYS	4.8
2	B	198	TYR	4.6
3	C	218	VAL	4.6
3	C	131	PRO	4.6
3	C	217	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
2	B	213	LYS	4.4
2	B	159	SER	3.9
2	B	122	SER	3.9
3	C	163	SER	3.8
2	B	211	ILE	3.8
2	B	208	THR	3.7
1	A	93	LYS	3.7
1	A	333	GLN	3.7
1	A	332	LEU	3.6
1	A	284	ILE	3.6
2	B	200	CYS	3.4
2	B	217	ARG	3.4
2	B	155	LYS	3.3
3	C	195	TRP	3.2
3	C	167	THR	3.2
2	B	190	ALA	3.2
2	B	119	PRO	3.1
3	C	1	GLN	3.1
3	C	216	LYS	3.1
3	C	145	LEU	3.1
2	B	154	TRP	3.1
1	A	8	ARG	3.1
2	B	158	GLY	3.1
2	B	166	LEU	3.1
2	B	193	GLU	3.0
2	B	194	ARG	3.0
3	C	166	LEU	3.0
2	B	201	GLU	3.0
2	B	192	TYR	3.0
2	B	197	LEU	2.9
1	A	108	TYR	2.9
2	B	137	THR	2.9
2	B	138	LEU	2.9
2	B	185	LEU	2.9
3	C	177	LEU	2.9
2	B	163	ASP	2.8
3	C	147	CYS	2.8
3	C	128	PRO	2.8
3	C	191	PRO	2.8
1	A	7	LYS	2.7
3	C	193	SER	2.7
2	B	149	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
3	C	64	LYS	2.7
3	C	130	ALA	2.7
2	B	195	HIS	2.7
2	B	131	LEU	2.6
3	C	151	GLY	2.6
2	B	187	LEU	2.6
2	B	161	LYS	2.6
1	A	168	ARG	2.6
3	C	44	LYS	2.5
3	C	168	SER	2.5
3	C	178	HIS	2.5
1	A	122	GLU	2.5
2	B	157	ASP	2.5
2	B	186	SER	2.5
1	A	202	GLY	2.5
2	B	212	VAL	2.5
3	C	141	ASN	2.4
3	C	63	LEU	2.4
2	B	202	VAL	2.4
2	B	133	THR	2.4
2	B	196	ASN	2.4
3	C	127	TYR	2.4
2	B	9	SER	2.4
2	B	132	GLY	2.4
3	C	165	ALA	2.4
2	B	216	ASN	2.3
2	B	124	PHE	2.3
2	B	164	GLY	2.3
3	C	161	TRP	2.2
3	C	200	VAL	2.2
3	C	205	ALA	2.2
2	B	148	LYS	2.2
1	A	114	MET	2.2
1	A	216	GLU	2.2
2	B	116	ASP	2.1
1	A	116	TYR	2.1
2	B	33	GLY	2.1
3	C	180	GLY	2.1
2	B	175	LYS	2.1
3	C	142	THR	2.1
2	B	206	THR	2.0
3	C	170	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SO4	A	346	5/5	0.49	0.16	158,158,159,159	0
5	SO4	A	344	5/5	0.63	0.17	155,156,156,156	0
4	GOL	B	221	6/6	0.64	0.24	125,127,127,127	0
5	SO4	C	224	5/5	0.64	0.10	178,178,179,179	0
4	GOL	A	338	6/6	0.65	0.15	110,112,112,113	0
5	SO4	A	343	5/5	0.71	0.11	154,154,155,155	0
5	SO4	A	340	5/5	0.71	0.11	145,145,145,145	0
4	GOL	A	337	6/6	0.73	0.30	102,105,106,107	0
4	GOL	A	336	6/6	0.73	0.18	77,79,83,85	0
5	SO4	A	345	5/5	0.74	0.13	136,137,138,138	0
5	SO4	A	348	5/5	0.75	0.11	155,155,156,156	0
5	SO4	C	223	5/5	0.77	0.54	71,71,71,71	5
5	SO4	C	222	5/5	0.78	0.24	78,78,80,80	5
4	GOL	A	335	6/6	0.80	0.28	101,102,104,106	0
5	SO4	B	223	5/5	0.81	0.59	34,35,36,37	5
5	SO4	A	347	5/5	0.81	0.22	75,75,76,76	5
5	SO4	B	222	5/5	0.83	0.15	76,76,77,78	5
5	SO4	A	350	5/5	0.83	0.13	97,99,99,101	0
5	SO4	B	224	5/5	0.83	0.22	143,143,143,144	0
5	SO4	A	349	5/5	0.84	0.09	147,148,148,148	0
5	SO4	A	341	5/5	0.84	0.12	137,138,139,139	0
6	AKG	A	600	10/10	0.84	0.30	125,131,133,133	0
7	FE	A	601	1/1	0.85	0.11	142,142,142,142	0
5	SO4	A	342	5/5	0.86	0.09	140,140,141,141	0
5	SO4	A	351	5/5	0.86	0.25	96,96,96,97	5
5	SO4	A	339	5/5	0.89	0.26	61,62,63,64	5
8	HG	A	352	1/1	0.96	0.11	98,98,98,98	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	HG	A	353	1/1	0.97	0.12	122,122,122,122	1

6.5 Other polymers [i](#)

There are no such residues in this entry.