



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 01:08 AM GMT

PDB ID : 2OCD
Title : Crystal structure of L-asparaginase I from *Vibrio cholerae* O1 biovar eltor str. N16961
Authors : Nocek, B.; Wu, R.; Osipiuk, J.; Moy, S.; Kim, Y.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2006-12-20
Resolution : 2.45 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

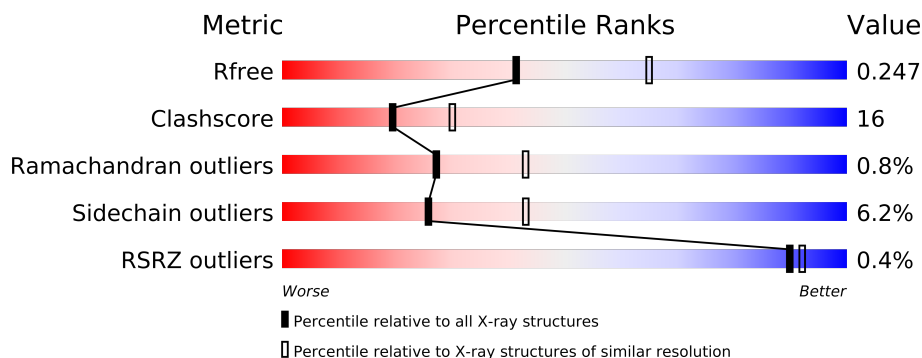
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.45 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}	66092	3566 (2.50-2.42)
Clashscore	79885	4471 (2.50-2.42)
Ramachandran outliers	78287	4383 (2.50-2.42)
Sidechain outliers	78261	4385 (2.50-2.42)
RSRZ outliers	66119	3568 (2.50-2.42)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	337	
1	B	337	
1	C	337	
1	D	337	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	ACT	B	602	-	X
2	ACT	C	604	-	X
3	GOL	D	605	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10702 atoms, of which 0 are hydrogen and 0 are deuterium.

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 L-asparaginase I.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	Se	0	1	0
			2513	1596	423	477	2	15			
1	B	333	Total	C	N	O	S	Se	0	5	0
			2579	1641	435	486	2	15			
1	C	328	Total	C	N	O	S	Se	0	1	0
			2512	1597	423	475	2	15			
1	D	332	Total	C	N	O	S	Se	0	2	0
			2552	1622	428	485	2	15			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
A	17	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
A	31	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
A	38	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
A	46	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
A	58	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
A	63	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
A	94	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
A	104	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
A	156	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
A	218	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
A	238	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
A	281	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
A	301	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
A	327	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
A	335	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
B	17	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
B	31	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
B	38	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
B	46	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3

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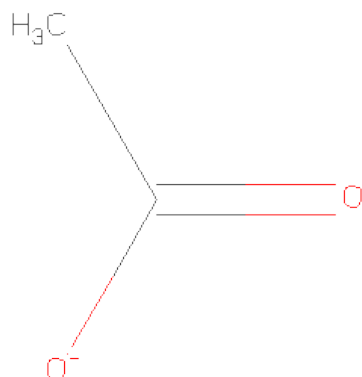
Chain	Residue	Modelled	Actual	Comment	Reference
B	58	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
B	63	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
B	94	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
B	104	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
B	156	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
B	218	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
B	238	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
B	281	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
B	301	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
B	327	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
B	335	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
C	17	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
C	31	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
C	38	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
C	46	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
C	58	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
C	63	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
C	94	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
C	104	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
C	156	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
C	218	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
C	238	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
C	281	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
C	301	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
C	327	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
C	335	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
D	17	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
D	31	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
D	38	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
D	46	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
D	58	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
D	63	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
D	94	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
D	104	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
D	156	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
D	218	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
D	238	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
D	281	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
D	301	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
D	327	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	335	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

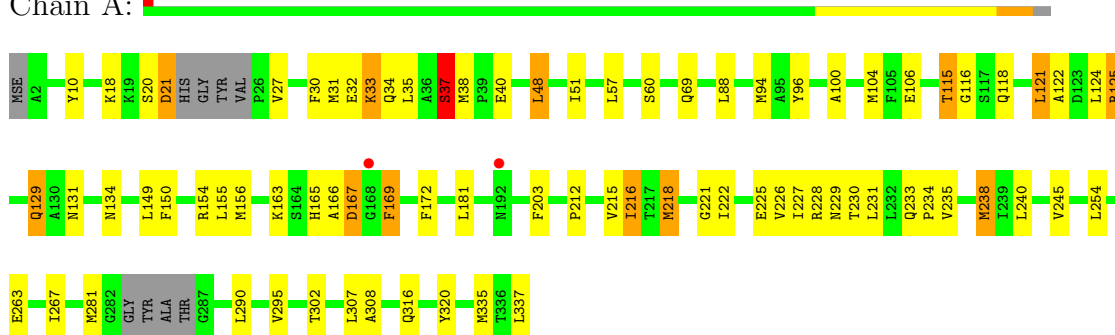
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	142	Total	O	0	0
			142	142		
4	B	126	Total	O	0	0
			126	126		
4	C	123	Total	O	0	0
			123	123		
4	D	133	Total	O	0	0
			133	133		

3 Residue-property plots

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

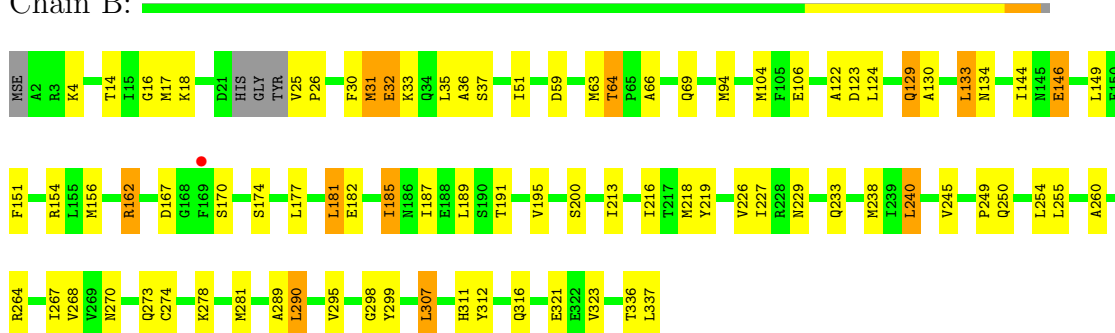
• Molecule 1: L-asparaginase I

Chain A:



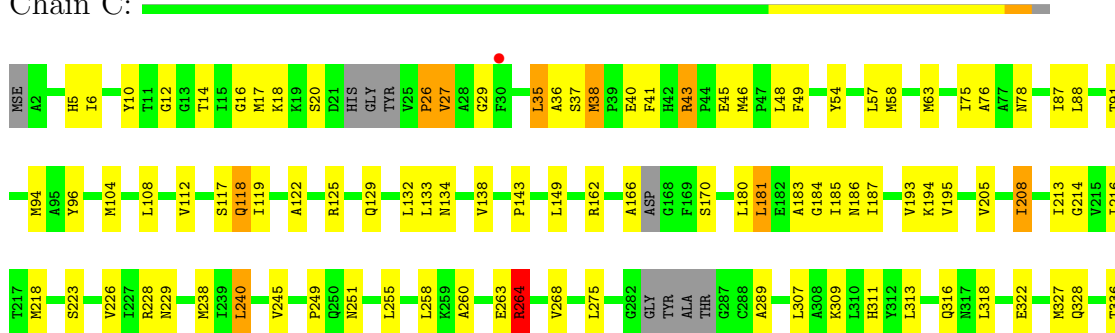
• Molecule 1: L-asparaginase I

Chain B:



• Molecule 1: L-asparaginase I

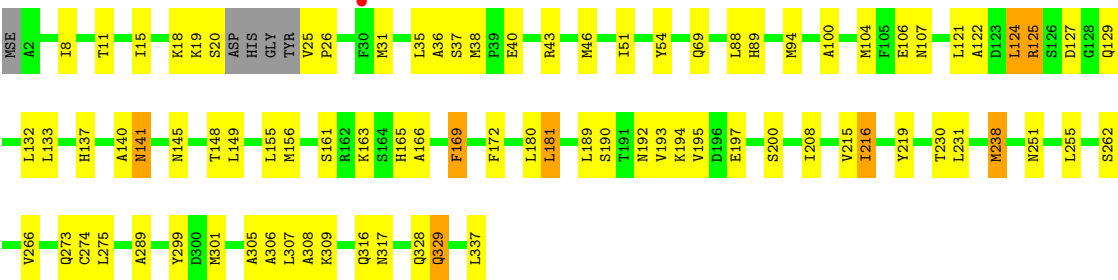
Chain C:



L337

● Molecule 1: L-asparaginase I

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.23Å 117.84Å 121.43Å 90.00° 91.44° 90.00°	Depositor
Resolution (Å)	33.30 – 2.45 33.36 – 2.45	Depositor EDS
% Data completeness (in resolution range)	97.4 (33.30-2.45) 97.2 (33.36-2.45)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.176 , 0.246 0.181 , 0.247	Depositor DCC
R_{free} test set	2741 reflections (5.39%)	DCC
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 22.0	EDS
Estimated twinning fraction	0.029 for -h,l,k 0.037 for -h,-l,-k 0.075 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 53624 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10702	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.90	0/2548	0.88	3/3429 (0.1%)
1	B	0.90	4/2622 (0.2%)	0.92	3/3530 (0.1%)
1	C	0.94	3/2546 (0.1%)	0.91	5/3426 (0.1%)
1	D	0.86	0/2590	0.88	1/3491 (0.0%)
All	All	0.90	7/10306 (0.1%)	0.90	12/13876 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	263	GLU	CG-CD	6.33	1.61	1.51
1	B	32	GLU	CD-OE2	-5.91	1.19	1.25
1	C	263	GLU	CB-CG	5.81	1.63	1.52
1	B	274	CYS	CB-SG	-5.69	1.72	1.81
1	B	123	ASP	CB-CG	5.42	1.63	1.51
1	C	322	GLU	CD-OE2	5.13	1.31	1.25
1	B	146	GLU	CG-CD	5.11	1.59	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	264	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	A	125	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	C	35	LEU	CA-CB-CG	6.70	130.71	115.30
1	A	48	LEU	CA-CB-CG	6.59	130.47	115.30
1	D	125	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	C	264	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	B	162	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	C	240	LEU	CA-CB-CG	5.27	127.43	115.30
1	C	43	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	A	48	LEU	CB-CG-CD2	-5.21	102.14	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	307	LEU	CA-CB-CG	-5.09	103.60	115.30
1	B	240	LEU	CB-CG-CD2	-5.09	102.35	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2513	0	2510	81	0
1	B	2579	0	2591	87	0
1	C	2512	0	2513	106	0
1	D	2552	0	2545	73	0
2	A	4	0	3	3	0
2	B	8	0	6	0	0
2	C	4	0	3	0	0
3	D	6	0	8	0	0
4	A	142	0	0	9	0
4	B	126	0	0	6	0
4	C	123	0	0	5	0
4	D	133	0	0	6	0
All	All	10702	0	10179	329	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (329) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:309:LYS:HG2	1:C:327:MSE:CE	1.85	1.05
1:C:58:MSE:HB3	1:C:63:MSE:HE2	1.36	1.04
1:A:165:HIS:ND1	1:A:169:PHE:CZ	2.26	1.02
1:B:124:LEU:HD21	1:D:46:MSE:HE3	1.43	1.01
1:C:309:LYS:CB	1:C:327:MSE:HE1	1.91	1.00
1:C:309:LYS:CG	1:C:327:MSE:HE1	1.92	1.00

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:75:ILE:HD11	1:C:87:ILE:HD11	1.43	0.99
1:C:309:LYS:HB3	1:C:327:MSE:HE1	1.44	0.97
1:C:216:ILE:HD11	1:C:240:LEU:CD2	1.95	0.96
1:C:58:MSE:CB	1:C:63:MSE:HE2	1.95	0.95
1:A:115:THR:HG23	1:A:150:PHE:O	1.69	0.93
1:C:313:LEU:HD12	1:C:327:MSE:HE3	1.50	0.91
1:B:25:VAL:HG23	1:B:26:PRO:HD3	1.54	0.90
1:C:216:ILE:HD11	1:C:240:LEU:HD22	1.53	0.88
1:D:19:LYS:NZ	1:D:25:VAL:HG23	1.89	0.88
1:A:218:MSE:HE2	1:A:222:ILE:HD13	1.55	0.88
1:C:309:LYS:CG	1:C:327:MSE:CE	2.49	0.87
1:B:25:VAL:HG23	1:B:26:PRO:CD	2.06	0.85
1:D:215:VAL:O	1:D:216:ILE:HD12	1.80	0.81
1:A:37[A]:SER:HB2	4:A:677:HOH:O	1.82	0.80
1:A:94:MSE:HE3	1:A:149:LEU:CG	2.15	0.76
1:B:267:ILE:HD13	1:B:323:VAL:CG1	2.16	0.76
1:B:94:MSE:CE	1:B:149:LEU:HD21	2.16	0.76
1:A:27:VAL:HG21	1:A:57:LEU:HD21	1.67	0.76
1:B:31:MSE:SE	1:B:35:LEU:HD11	2.36	0.76
1:D:35:LEU:HD11	1:D:122:ALA:HB2	1.68	0.76
1:A:27:VAL:HG21	1:A:57:LEU:CD2	2.17	0.75
1:D:25:VAL:O	1:D:25:VAL:HG22	1.86	0.75
1:B:227:ILE:HD12	1:B:254:LEU:HD11	1.68	0.75
1:A:94:MSE:HE3	1:A:149:LEU:HG	1.69	0.74
1:C:91:THR:HA	1:C:94:MSE:HE3	1.68	0.74
1:C:38:MSE:HB2	4:C:687:HOH:O	1.86	0.73
1:C:216:ILE:HD11	1:C:240:LEU:HD23	1.70	0.73
1:C:134:ASN:O	1:C:138:VAL:HG23	1.88	0.73
1:C:75:ILE:CD1	1:C:87:ILE:HD11	2.18	0.73
1:C:12:GLY:HA2	1:C:57:LEU:HD22	1.68	0.73
1:C:38:MSE:CE	1:C:129:GLN:HE22	2.02	0.72
1:C:27:VAL:HG11	1:C:57:LEU:CD1	2.18	0.72
1:A:226:VAL:O	1:A:230:THR:HG23	1.90	0.72
1:B:185:ILE:HG22	1:D:169:PHE:CD1	2.25	0.71
1:A:48:LEU:HD12	4:A:606:HOH:O	1.88	0.71
1:B:25:VAL:CG2	1:B:26:PRO:HD3	2.21	0.70
1:D:19:LYS:HZ1	1:D:25:VAL:HG23	1.56	0.70
1:A:218:MSE:CE	1:A:222:ILE:HD13	2.21	0.70
1:A:125:ARG:HD2	1:C:134:ASN:OD1	1.92	0.69
1:D:141:ASN:N	1:D:141:ASN:HD22	1.90	0.69
1:C:216:ILE:O	1:C:216:ILE:HD12	1.92	0.69
1:B:227:ILE:CD1	1:B:254:LEU:HD11	2.23	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:218:MSE:CE	1:C:249:PRO:HD2	2.23	0.69
1:B:94:MSE:HE3	1:B:149:LEU:CG	2.23	0.68
1:B:250:GLN:O	1:B:250:GLN:HG3	1.93	0.68
1:D:19:LYS:HZ2	1:D:25:VAL:HG23	1.56	0.68
1:C:27:VAL:HG11	1:C:57:LEU:HD12	1.75	0.68
1:A:40:GLU:OE2	1:A:129:GLN:NE2	2.27	0.67
1:B:216:ILE:HD13	1:B:227:ILE:HG12	1.76	0.67
1:C:35:LEU:HD21	1:C:122:ALA:HB2	1.76	0.67
1:A:218:MSE:HE2	1:A:222:ILE:HG21	1.77	0.67
1:B:94:MSE:HE3	1:B:149:LEU:HG	1.77	0.67
1:D:156:MSE:HE1	1:D:172:PHE:HB2	1.77	0.67
1:B:255:LEU:HD21	1:B:289:ALA:HB1	1.77	0.67
1:B:267:ILE:HD13	1:B:323:VAL:HG12	1.77	0.66
1:C:104:MSE:CG	1:C:208:ILE:HD12	2.25	0.66
1:B:278:LYS:NZ	1:B:337:LEU:HD23	2.11	0.66
1:B:94:MSE:HE3	1:B:149:LEU:CD2	2.25	0.66
1:B:213:ILE:HD12	1:B:311:HIS:CE1	2.30	0.66
1:B:267:ILE:CD1	1:B:323:VAL:CG1	2.74	0.65
1:A:96:TYR:OH	1:B:273:GLN:NE2	2.28	0.65
1:C:309:LYS:HG2	1:C:327:MSE:HE2	1.77	0.65
1:A:165:HIS:ND1	1:A:169:PHE:CE2	2.58	0.65
1:A:216:ILE:HG21	1:A:218:MSE:HE1	1.79	0.65
1:A:134:ASN:HD21	1:C:125:ARG:HH21	1.46	0.64
1:B:25:VAL:N	4:B:721:HOH:O	2.31	0.64
1:C:27:VAL:CG1	1:C:57:LEU:CD1	2.75	0.64
1:D:46:MSE:HE2	1:D:46:MSE:HA	1.80	0.63
1:A:94:MSE:CE	1:A:149:LEU:HD21	2.28	0.63
1:B:154:ARG:HG3	1:B:156:MSE:HE2	1.81	0.63
1:B:267:ILE:HD13	1:B:323:VAL:HG11	1.80	0.63
1:B:245:VAL:O	1:B:245:VAL:HG12	1.98	0.63
1:A:181:LEU:C	1:A:181:LEU:HD23	2.19	0.63
1:B:278:LYS:HZ1	1:B:337:LEU:HD23	1.64	0.62
1:C:255:LEU:CD1	1:C:289:ALA:HB1	2.30	0.62
1:C:245:VAL:O	1:C:245:VAL:HG12	1.99	0.62
1:B:35:LEU:HD21	1:B:122:ALA:HB2	1.82	0.62
1:A:35:LEU:HD11	1:A:122:ALA:HB2	1.80	0.62
1:C:309:LYS:HG2	1:C:327:MSE:HE1	1.58	0.62
1:D:46:MSE:HE1	1:D:137:HIS:HB2	1.80	0.61
1:B:94:MSE:HE3	1:B:149:LEU:HD21	1.82	0.61
1:B:35:LEU:O	1:B:37[A]:SER:N	2.34	0.60
1:C:309:LYS:HE2	1:C:327:MSE:HE2	1.83	0.60
1:B:17:MSE:SE	1:B:25:VAL:O	2.69	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:307:LEU:HD21	1:D:219:TYR:HB2	1.84	0.60
1:B:267:ILE:CD1	1:B:323:VAL:HG11	2.32	0.60
1:D:106[A]:GLU:HG2	1:D:107:ASN:ND2	2.17	0.59
1:A:254:LEU:HD23	1:A:254:LEU:C	2.23	0.59
1:B:33[A]:LYS:HD3	1:B:51:ILE:CG2	2.32	0.59
1:C:328:GLN:NE2	4:C:658:HOH:O	2.34	0.59
1:D:149:LEU:HD23	1:D:149:LEU:C	2.23	0.59
1:B:336:THR:CG2	4:B:720:HOH:O	2.51	0.58
1:C:27:VAL:CG1	1:C:57:LEU:HD12	2.33	0.58
1:B:245:VAL:CG1	1:B:245:VAL:O	2.51	0.58
1:C:108:LEU:HD21	1:C:112:VAL:HG23	1.85	0.58
1:A:163:LYS:HE2	1:A:166:ALA:HB2	1.85	0.58
1:D:163:LYS:HZ2	1:D:166:ALA:HB2	1.68	0.58
1:C:183:ALA:HA	1:C:187:ILE:HD13	1.86	0.58
1:B:218:MSE:HE2	1:B:240:LEU:HG	1.84	0.57
1:B:249:PRO:O	1:B:250:GLN:HG2	2.05	0.57
1:B:144:ILE:HG22	1:B:146:GLU:HG3	1.86	0.57
1:C:58:MSE:HB2	1:C:63:MSE:HE2	1.86	0.57
1:A:121:LEU:O	1:A:121:LEU:HD23	2.03	0.57
1:B:290:LEU:HB2	4:B:685:HOH:O	2.04	0.57
1:C:63:MSE:HE3	4:C:628:HOH:O	2.05	0.57
1:B:185:ILE:CG2	1:D:169:PHE:CD1	2.89	0.56
1:A:316:GLN:HG3	4:A:684:HOH:O	2.05	0.56
1:D:8:ILE:HG21	1:D:51:ILE:HD12	1.85	0.56
1:C:255:LEU:HD13	1:C:289:ALA:HB1	1.86	0.56
1:C:38:MSE:CE	1:C:129:GLN:NE2	2.68	0.56
1:B:64:THR:HG22	1:B:66:ALA:N	2.20	0.56
1:B:336:THR:HG21	4:B:720:HOH:O	2.04	0.56
1:D:163:LYS:NZ	1:D:166:ALA:HB2	2.21	0.56
1:D:299:TYR:HE1	1:D:337:LEU:HD23	1.69	0.56
1:B:35:LEU:O	1:B:37[B]:SER:N	2.38	0.56
1:D:148:THR:OG1	1:D:155:LEU:HD11	2.06	0.56
1:C:41:PHE:CE1	1:C:133:LEU:HD13	2.41	0.56
1:A:38:MSE:HE1	1:A:121:LEU:HD21	1.88	0.56
1:A:38:MSE:HE2	1:A:129:GLN:HE21	1.71	0.55
1:C:18:LYS:O	1:C:26:PRO:HD2	2.06	0.55
1:C:218:MSE:HE3	1:C:249:PRO:HD2	1.87	0.55
1:D:25:VAL:O	1:D:25:VAL:CG2	2.55	0.55
1:A:216:ILE:CG2	1:A:218:MSE:HE3	2.37	0.55
1:A:216:ILE:HD11	1:A:230:THR:HG21	1.89	0.55
1:D:215:VAL:O	1:D:216:ILE:CD1	2.53	0.55
1:C:218:MSE:HE3	1:C:249:PRO:CD	2.37	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:35:LEU:O	1:D:37:SER:N	2.40	0.55
1:D:141:ASN:ND2	1:D:141:ASN:N	2.55	0.55
1:C:78:ASN:ND2	4:C:619:HOH:O	2.41	0.54
1:A:307:LEU:HD21	1:B:219:TYR:HB2	1.89	0.54
1:A:69:GLN:HA	1:A:104:MSE:HE1	1.90	0.54
1:D:104:MSE:HE3	1:D:208:ILE:HG22	1.90	0.54
1:A:100:ALA:HA	1:A:308:ALA:HB1	1.88	0.54
1:C:260:ALA:O	1:C:264:ARG:HG2	2.07	0.54
1:C:17:MSE:HE2	1:C:27:VAL:HG13	1.90	0.54
1:C:245:VAL:CG1	1:C:245:VAL:O	2.55	0.54
1:C:96:TYR:OH	1:D:273:GLN:NE2	2.38	0.54
1:A:94:MSE:HE3	1:A:149:LEU:CD2	2.38	0.54
1:D:181:LEU:C	1:D:181:LEU:HD23	2.29	0.53
1:B:129:GLN:O	1:B:133:LEU:HB2	2.09	0.53
1:C:27:VAL:HG11	1:C:57:LEU:HD13	1.88	0.53
1:A:134:ASN:ND2	1:C:125:ARG:HH21	2.06	0.53
1:A:216:ILE:CG2	1:A:218:MSE:CE	2.86	0.53
1:C:35:LEU:O	1:C:37[B]:SER:N	2.42	0.53
1:A:267:ILE:HD13	1:A:320:TYR:CE1	2.44	0.53
1:B:16:GLY:CA	1:B:32:GLU:HG2	2.39	0.53
1:D:299:TYR:CE1	1:D:337:LEU:HD23	2.43	0.52
1:D:216:ILE:HD13	1:D:230:THR:HG21	1.92	0.52
1:B:278:LYS:HZ1	1:B:337:LEU:CD2	2.22	0.52
1:B:64:THR:CG2	1:B:66:ALA:H	2.22	0.52
1:B:69:GLN:HA	1:B:104:MSE:HE1	1.92	0.52
1:A:238:MSE:HE1	1:A:240:LEU:HD21	1.92	0.52
1:A:60:SER:CB	2:A:601:ACT:H1	2.38	0.52
1:A:169:PHE:O	1:A:169:PHE:CG	2.63	0.52
1:B:189:LEU:HD21	1:B:195:VAL:HG23	1.92	0.51
1:C:35:LEU:O	1:C:37[A]:SER:N	2.43	0.51
1:A:34:GLN:NE2	4:A:710:HOH:O	2.42	0.51
1:C:43:ARG:HD3	1:C:45:GLU:OE1	2.11	0.51
1:A:60:SER:HB2	2:A:601:ACT:H1	1.92	0.51
1:A:37[A]:SER:CB	4:A:677:HOH:O	2.49	0.51
1:B:321:GLU:HG2	4:B:657:HOH:O	2.11	0.51
1:B:59:ASP:C	1:B:59:ASP:OD1	2.50	0.50
1:C:88:LEU:HD21	1:C:132:LEU:HD13	1.92	0.50
1:C:214:GLY:HA3	1:C:238:MSE:CE	2.41	0.50
1:B:216:ILE:CD1	1:B:238:MSE:SE	3.10	0.50
1:C:38:MSE:HE2	1:C:129:GLN:HE22	1.76	0.50
1:A:115:THR:HG21	1:A:131:ASN:HB3	1.92	0.50
1:A:216:ILE:HG21	1:A:218:MSE:CE	2.42	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:165:HIS:HB3	1:A:169:PHE:CE1	2.47	0.49
1:B:278:LYS:HZ2	1:B:337:LEU:HG	1.77	0.49
1:D:100:ALA:HA	1:D:308:ALA:HB1	1.93	0.49
1:A:115:THR:HG22	1:A:116:GLY:H	1.77	0.49
1:C:6:ILE:O	1:C:49:PHE:HA	2.13	0.49
1:A:234:PRO:O	1:A:235:VAL:C	2.51	0.49
1:C:213:ILE:HD12	1:C:311:HIS:CE1	2.48	0.49
1:B:16:GLY:HA2	1:B:32:GLU:HG2	1.94	0.49
1:B:268:VAL:HG12	1:B:295:VAL:HG13	1.93	0.49
1:D:301:MSE:HG3	1:D:305:ALA:HB3	1.94	0.49
1:B:216:ILE:HG13	1:B:238:MSE:SE	2.63	0.49
1:D:140:ALA:C	1:D:141:ASN:HD22	2.15	0.49
1:A:33:LYS:HB2	1:A:33:LYS:HZ3	1.78	0.49
1:B:17:MSE:CE	1:B:25:VAL:O	2.61	0.48
1:C:20:SER:CB	1:C:26:PRO:HD3	2.43	0.48
1:D:46:MSE:HE1	1:D:137:HIS:CB	2.44	0.48
1:C:104:MSE:HG3	1:C:208:ILE:HD12	1.95	0.48
1:D:35:LEU:C	1:D:37:SER:H	2.17	0.48
1:C:166:ALA:HB2	1:D:274:CYS:SG	2.54	0.48
1:D:189:LEU:HD11	1:D:195:VAL:CG2	2.44	0.48
1:A:37[B]:SER:N	4:A:677:HOH:O	2.47	0.48
1:C:35:LEU:C	1:C:37[B]:SER:H	2.17	0.48
1:B:25:VAL:HG23	1:B:26:PRO:HD2	1.94	0.48
1:B:278:LYS:NZ	1:B:337:LEU:CD2	2.76	0.48
1:B:33[A]:LYS:HD3	1:B:51:ILE:HG21	1.96	0.48
1:D:145:ASN:ND2	1:D:197:GLU:O	2.43	0.48
1:A:94:MSE:HE3	1:A:149:LEU:HD21	1.96	0.47
1:B:185:ILE:HD12	1:D:127:ASP:HB3	1.96	0.47
1:D:165:HIS:CD2	4:D:674:HOH:O	2.67	0.47
1:B:64:THR:CG2	1:B:66:ALA:HB3	2.45	0.47
1:C:181:LEU:HD23	1:C:181:LEU:C	2.35	0.47
1:C:264:ARG:NH2	4:C:722:HOH:O	2.47	0.47
1:A:60:SER:H	2:A:601:ACT:H1	1.79	0.47
1:D:40:GLU:HB3	4:D:638:HOH:O	2.14	0.47
1:B:267:ILE:CD1	1:B:323:VAL:HG12	2.44	0.47
1:D:35:LEU:CD1	1:D:122:ALA:HB2	2.43	0.47
1:D:104:MSE:HE3	1:D:208:ILE:CG2	2.44	0.47
1:C:35:LEU:C	1:C:37[A]:SER:H	2.19	0.46
1:C:307:LEU:HD21	1:D:219:TYR:CB	2.45	0.46
1:A:106:GLU:O	1:A:203:PHE:HA	2.15	0.46
1:C:255:LEU:HD11	1:C:289:ALA:HB1	1.96	0.46
1:C:309:LYS:CD	1:C:327:MSE:HE2	2.46	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:134:ASN:OD1	1:D:125:ARG:HD2	2.16	0.46
1:A:30:PHE:HB3	4:A:709:HOH:O	2.15	0.46
1:C:143:PRO:HD2	1:C:195:VAL:HG13	1.98	0.46
1:C:216:ILE:HG13	1:C:238:MSE:SE	2.65	0.46
1:B:278:LYS:NZ	1:B:337:LEU:HG	2.30	0.46
1:A:169:PHE:O	1:A:169:PHE:CD1	2.69	0.46
1:C:134:ASN:O	1:C:138:VAL:CG2	2.62	0.46
1:D:40:GLU:OE2	1:D:129:GLN:NE2	2.49	0.46
1:A:229:ASN:O	1:B:229:ASN:HB3	2.16	0.46
1:D:18:LYS:O	1:D:26:PRO:HD2	2.15	0.46
1:C:149:LEU:C	1:C:149:LEU:HD23	2.37	0.46
1:D:25:VAL:N	1:D:26:PRO:HD3	2.31	0.46
1:A:216:ILE:HG22	1:A:218:MSE:HE3	1.97	0.46
1:A:231:LEU:CD2	1:A:238:MSE:HG3	2.46	0.45
1:B:187:ILE:HD12	1:D:125:ARG:NH2	2.32	0.45
1:C:5:HIS:HA	1:C:48:LEU:O	2.16	0.45
1:D:255:LEU:HD11	1:D:289:ALA:HB1	1.98	0.45
1:B:312:TYR:O	1:B:316:GLN:NE2	2.49	0.45
1:B:336:THR:O	1:B:337:LEU:HB2	2.16	0.45
1:C:20:SER:HB3	1:C:26:PRO:HD3	1.99	0.45
1:D:301:MSE:HG2	1:D:306:ALA:HB2	1.98	0.45
1:C:316:GLN:HB2	1:C:318:LEU:HG	1.99	0.45
1:D:149:LEU:HD13	1:D:161:SER:OG	2.17	0.45
1:B:181:LEU:HD12	1:B:182:GLU:N	2.32	0.45
1:C:313:LEU:HD12	1:C:327:MSE:CE	2.35	0.45
1:D:43:ARG:HD2	4:D:737:HOH:O	2.16	0.45
1:C:313:LEU:CD1	1:C:327:MSE:HE3	2.34	0.44
1:B:250:GLN:CG	1:B:250:GLN:O	2.62	0.44
1:B:298:GLY:O	1:B:299:TYR:C	2.56	0.44
1:C:118:GLN:HE22	1:C:170:SER:H	1.66	0.44
1:A:216:ILE:HD13	1:A:216:ILE:HA	1.77	0.44
1:C:38:MSE:HE2	1:C:129:GLN:NE2	2.32	0.44
1:B:181:LEU:HD12	1:B:181:LEU:C	2.38	0.44
1:D:251:ASN:HB2	4:D:627:HOH:O	2.17	0.44
1:B:260:ALA:O	1:B:264[B]:ARG:HG2	2.18	0.44
1:C:309:LYS:CD	1:C:327:MSE:CE	2.96	0.43
1:B:25:VAL:CB	1:B:26:PRO:HD3	2.48	0.43
1:D:20:SER:N	1:D:25:VAL:N	2.65	0.43
1:B:129:GLN:HG3	1:B:130:ALA:N	2.33	0.43
1:C:54:TYR:HD2	1:C:58:MSE:HE3	1.82	0.43
1:A:94:MSE:HE3	1:A:149:LEU:CD1	2.48	0.43
1:A:212:PRO:O	1:A:235:VAL:HA	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:89:HIS:O	1:D:94:MSE:HE2	2.18	0.43
1:D:88:LEU:HD21	1:D:132:LEU:HD13	2.00	0.43
1:D:208:ILE:O	1:D:208:ILE:HG23	2.18	0.43
1:B:129:GLN:HE21	1:B:129:GLN:HB2	1.69	0.43
1:A:302:THR:HG23	4:A:604:HOH:O	2.18	0.43
1:D:316:GLN:NE2	4:D:620:HOH:O	2.51	0.43
1:C:214:GLY:HA3	1:C:238:MSE:HE1	2.01	0.43
1:A:27:VAL:HG11	1:A:57:LEU:CD2	2.49	0.43
1:A:125:ARG:NH2	1:C:184:GLY:O	2.39	0.43
1:A:20:SER:OG	1:A:21:ASP:N	2.51	0.43
1:B:278:LYS:NZ	1:B:337:LEU:CG	2.82	0.43
1:D:8:ILE:CG2	1:D:51:ILE:HD12	2.49	0.43
1:D:11:THR:HG22	1:D:54:TYR:CE2	2.54	0.43
1:A:227:ILE:HD13	1:A:227:ILE:N	2.34	0.42
1:C:27:VAL:CG1	1:C:57:LEU:HD13	2.48	0.42
1:D:180:LEU:O	1:D:193:VAL:HG21	2.18	0.42
1:D:149:LEU:HD22	1:D:156:MSE:HE3	2.00	0.42
1:A:281:MSE:HE3	1:A:290:LEU:HB2	2.01	0.42
1:C:216:ILE:C	1:C:216:ILE:HD12	2.39	0.42
1:A:118:GLN:NE2	4:A:614:HOH:O	2.51	0.42
1:C:275:LEU:HD22	1:D:275:LEU:HD22	2.00	0.42
1:C:228:ARG:NH2	1:C:229:ASN:OD1	2.53	0.42
1:B:14:THR:HG23	1:B:17:MSE:HE2	2.01	0.42
1:C:208:ILE:HG22	1:C:208:ILE:O	2.19	0.42
1:B:16:GLY:HA3	1:B:32:GLU:HG2	2.00	0.42
1:D:40:GLU:HG3	1:D:133:LEU:HD11	2.00	0.42
1:C:238:MSE:HG3	1:C:268:VAL:HG13	2.01	0.42
1:A:37[B]:SER:OG	1:A:37[B]:SER:O	2.29	0.42
1:B:64:THR:CG2	1:B:66:ALA:N	2.81	0.42
1:B:64:THR:HG22	1:B:66:ALA:HB3	2.00	0.42
1:A:290:LEU:HD22	1:A:295:VAL:HG21	2.01	0.42
1:D:231:LEU:HG	1:D:238:MSE:HE2	2.01	0.42
1:B:94:MSE:HE2	1:B:149:LEU:HD21	2.00	0.42
1:A:231:LEU:HD21	1:A:238:MSE:HG3	2.01	0.42
1:C:327:MSE:HA	1:C:327:MSE:HE2	2.01	0.42
1:D:262:SER:HA	1:D:266:VAL:O	2.20	0.42
1:C:133:LEU:HD12	1:C:133:LEU:HA	1.95	0.41
1:A:156:MSE:HE1	1:A:172:PHE:HB2	2.02	0.41
1:A:335:MSE:HE3	1:A:337:LEU:HD21	2.01	0.41
1:C:228:ARG:CZ	1:C:228:ARG:HB3	2.51	0.41
1:C:185:ILE:HG23	1:C:186:ASN:ND2	2.34	0.41
1:C:76:ALA:HB2	1:C:205:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:117:SER:OG	1:C:119:ILE:O	2.30	0.41
1:B:233:GLN:NE2	4:B:677:HOH:O	2.52	0.41
1:A:38:MSE:CE	1:A:129:GLN:HE21	2.32	0.41
1:A:225:GLU:HG3	1:A:228:ARG:NH2	2.35	0.41
1:A:94:MSE:CE	1:A:149:LEU:HD11	2.50	0.41
1:B:270:ASN:HD22	1:B:281:MSE:SE	2.53	0.41
1:C:180:LEU:HD22	1:C:193:VAL:HG22	2.01	0.41
1:C:309:LYS:HE2	1:C:327:MSE:HA	2.02	0.41
1:A:215:VAL:O	1:A:216:ILE:HD13	2.21	0.41
1:A:221:GLY:O	1:A:222:ILE:C	2.58	0.41
1:A:169:PHE:N	1:A:169:PHE:CD1	2.89	0.41
1:C:214:GLY:HA3	1:C:238:MSE:HE2	2.03	0.41
1:D:69:GLN:HA	1:D:104:MSE:HE1	2.02	0.41
1:D:121:LEU:HG	1:D:121:LEU:O	2.20	0.41
1:D:309:LYS:NZ	1:D:329:GLN:O	2.46	0.41
1:D:124:LEU:O	1:D:124:LEU:HD23	2.21	0.41
1:C:309:LYS:CE	1:C:327:MSE:HE2	2.48	0.41
1:B:154:ARG:CG	1:B:156:MSE:HE2	2.48	0.41
1:C:46:MSE:HE2	1:C:133:LEU:HD12	2.03	0.41
1:A:10:TYR:HA	1:A:88:LEU:HB2	2.03	0.40
1:C:216:ILE:CD1	1:C:240:LEU:HD23	2.47	0.40
1:B:31:MSE:O	1:B:35:LEU:HD13	2.22	0.40
1:A:155:LEU:HB3	1:A:181:LEU:HB3	2.03	0.40
1:D:190:SER:OG	1:D:193:VAL:HG23	2.22	0.40
1:D:328:GLN:NE2	4:D:628:HOH:O	2.44	0.40
1:C:10:TYR:CZ	1:C:16:GLY:HA3	2.55	0.40
1:C:309:LYS:CG	1:C:327:MSE:HE2	2.39	0.40
1:C:143:PRO:HD2	1:C:195:VAL:CG1	2.51	0.40
1:A:222:ILE:CD1	1:A:227:ILE:HD11	2.51	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	323/337 (96%)	310 (96%)	9 (3%)	4 (1%)	19	30
1	B	334/337 (99%)	312 (93%)	19 (6%)	3 (1%)	25	39
1	C	321/337 (95%)	303 (94%)	15 (5%)	3 (1%)	25	39
1	D	330/337 (98%)	311 (94%)	17 (5%)	2 (1%)	33	52
All	All	1308/1348 (97%)	1236 (94%)	60 (5%)	12 (1%)	27	39

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37[A]	SER
1	A	37[B]	SER
1	B	36	ALA
1	B	167	ASP
1	C	26	PRO
1	C	29	GLY
1	C	36	ALA
1	D	36	ALA
1	D	200	SER
1	B	63	MSE
1	A	167	ASP
1	A	245	VAL

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	273/262 (104%)	253 (93%)	20 (7%)	20	34
1	B	280/262 (107%)	259 (92%)	21 (8%)	19	32
1	C	273/262 (104%)	258 (94%)	15 (6%)	30	50
1	D	276/262 (105%)	262 (95%)	14 (5%)	33	55
All	All	1102/1048 (105%)	1032 (94%)	70 (6%)	26	41

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LYS
1	A	21	ASP
1	A	31	MSE
1	A	32	GLU
1	A	33	LYS
1	A	37[A]	SER
1	A	37[B]	SER
1	A	51	ILE
1	A	115	THR
1	A	121	LEU
1	A	124	LEU
1	A	129	GLN
1	A	154	ARG
1	A	167	ASP
1	A	169	PHE
1	A	216	ILE
1	A	218	MSE
1	A	233	GLN
1	A	238	MSE
1	A	263	GLU
1	B	4[A]	LYS
1	B	4[B]	LYS
1	B	18	LYS
1	B	30	PHE
1	B	31	MSE
1	B	64	THR
1	B	106	GLU
1	B	129	GLN
1	B	133	LEU
1	B	151	PHE
1	B	162	ARG
1	B	170	SER
1	B	174	SER
1	B	177	LEU
1	B	181	LEU
1	B	185	ILE
1	B	191	THR
1	B	200	SER
1	B	226	VAL
1	B	290	LEU
1	B	307	LEU
1	C	14	THR
1	C	27	VAL

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Mol	Chain	Res	Type
1	C	38	MSE
1	C	40	GLU
1	C	118	GLN
1	C	162	ARG
1	C	181	LEU
1	C	194	LYS
1	C	208	ILE
1	C	223	SER
1	C	226	VAL
1	C	251	ASN
1	C	258	LEU
1	C	264	ARG
1	C	336	THR
1	D	15	ILE
1	D	31	MSE
1	D	38	MSE
1	D	124	LEU
1	D	141	ASN
1	D	169	PHE
1	D	181	LEU
1	D	192	ASN
1	D	194	LYS
1	D	216	ILE
1	D	238	MSE
1	D	307	LEU
1	D	317	ASN
1	D	329	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	118	GLN
1	A	129	GLN
1	A	186	ASN
1	A	257	GLN
1	A	316	GLN
1	B	129	GLN
1	B	131	ASN
1	B	145	ASN
1	B	251	ASN
1	B	273	GLN

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Mol	Chain	Res	Type
1	B	316	GLN
1	C	78	ASN
1	C	118	GLN
1	C	129	GLN
1	C	141	ASN
1	C	145	ASN
1	C	186	ASN
1	C	247	ASN
1	C	251	ASN
1	C	273	GLN
1	C	280	ASN
1	C	316	GLN
1	D	107	ASN
1	D	141	ASN
1	D	165	HIS
1	D	192	ASN
1	D	224	HIS
1	D	250	GLN
1	D	257	GLN
1	D	273	GLN
1	D	316	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

5 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	ACT	A	601	-	1,3,3	2.43	1 (100%)	0,3,3	0.00	-
2	ACT	B	602	-	1,3,3	1.80	0	0,3,3	0.00	-
2	ACT	B	603	-	1,3,3	1.94	0	0,3,3	0.00	-
2	ACT	C	604	-	1,3,3	2.56	1 (100%)	0,3,3	0.00	-
3	GOL	D	605	-	5,5,5	0.33	0	5,5,5	0.46	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	ACT	A	601	-	-	0/0/0/0	0/0/0/0
2	ACT	B	602	-	-	0/0/0/0	0/0/0/0
2	ACT	B	603	-	-	0/0/0/0	0/0/0/0
2	ACT	C	604	-	-	0/0/0/0	0/0/0/0
3	GOL	D	605	-	-	0/4/4/4	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	604	ACT	CH3-C	2.56	1.52	1.48
2	A	601	ACT	CH3-C	2.43	1.52	1.48

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	328/337 (97%)	-0.63	2 (0%) 86 88	5, 16, 32, 41	2 (0%)
1	B	333/337 (98%)	-0.61	1 (0%) 91 94	9, 18, 34, 42	2 (0%)
1	C	328/337 (97%)	-0.61	1 (0%) 91 94	6, 16, 32, 56	1 (0%)
1	D	332/337 (98%)	-0.60	1 (0%) 91 94	7, 18, 36, 41	0
All	All	1321/1348 (97%)	-0.61	5 (0%) 90 92	5, 17, 34, 56	5 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	30	PHE	2.7
1	A	192	ASN	2.6
1	B	169	PHE	2.5
1	A	168	GLY	2.4
1	C	30	PHE	2.2

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 carbohydrates 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. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	GOL	D	605	6/6	0.22	7.83	63,64,64,65	0
2	ACT	B	602	4/4	0.17	3.79	54,54,54,54	0
2	ACT	C	604	4/4	0.15	2.60	47,48,49,49	0
2	ACT	A	601	4/4	0.13	0.92	37,38,38,39	0
2	ACT	B	603	4/4	0.10	0.05	51,51,51,51	0

6.5 Other polymers ⓘ

There are no such residues in this entry.