



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:31 pm 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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

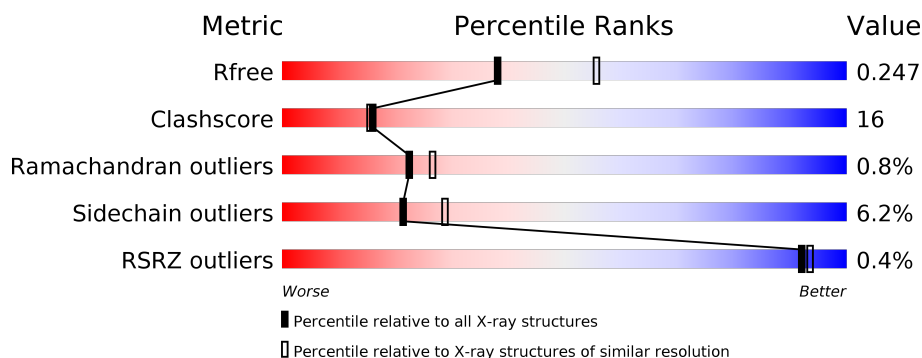
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	100719	1119 (2.48-2.44)
Clashscore	112137	1193 (2.48-2.44)
Ramachandran outliers	110173	1185 (2.48-2.44)
Sidechain outliers	110143	1185 (2.48-2.44)
RSRZ outliers	101464	1126 (2.48-2.44)

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  $\geq 3$ , 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	337	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>74%</span> <span>20%</span> </div> </div>
1	B	337	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>73%</span> <span>22%</span> </div> </div>
1	C	337	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>69%</span> <span>26%</span> </div> </div>
1	D	337	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>73%</span> <span>23%</span> </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	ACT	A	601	-	-	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 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 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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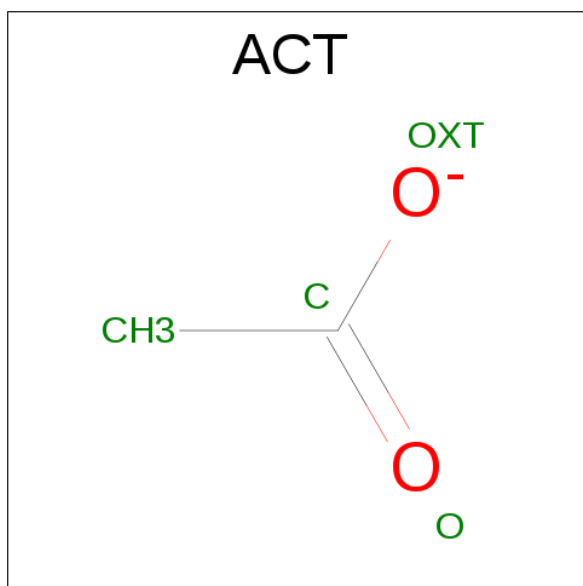
Chain	Residue	Modelled	Actual	Comment	Reference
B	58	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
B	63	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
B	94	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
B	104	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
B	156	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
B	218	MSE	MET	MODIFIED RESIDUE	UNP Q9KQK3
B	238	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		

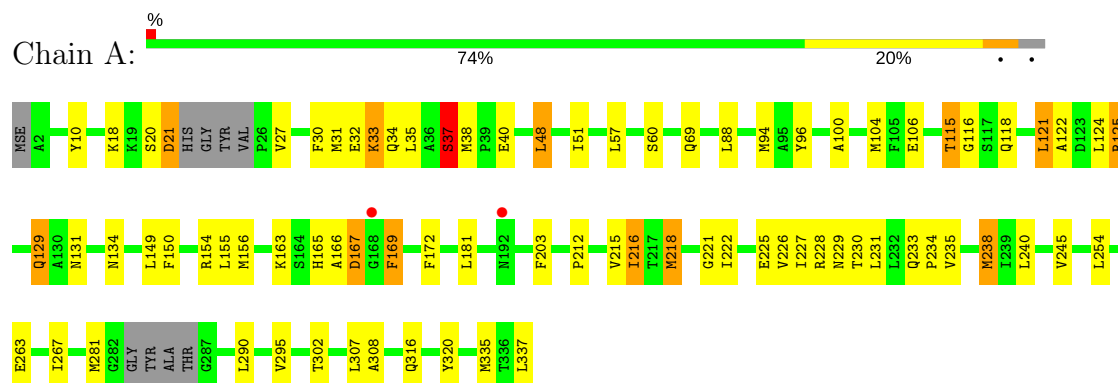
- Molecule 4 is water.

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		

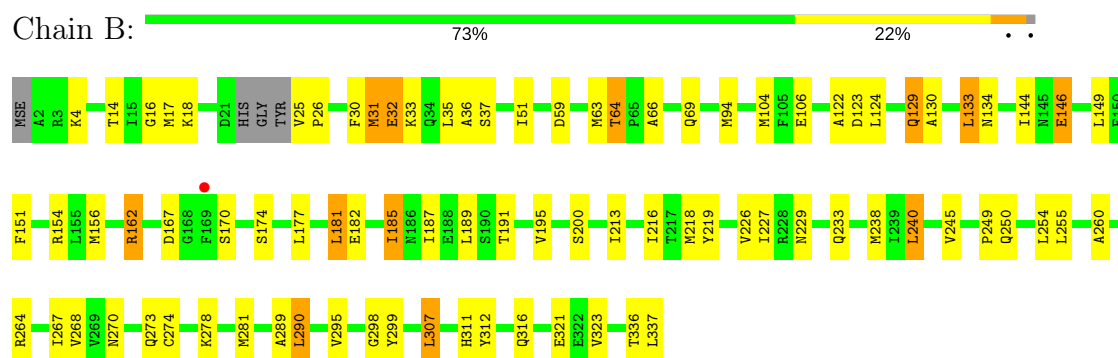
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: L-asparaginase I



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#### • Molecule 1: L-asparaginase I





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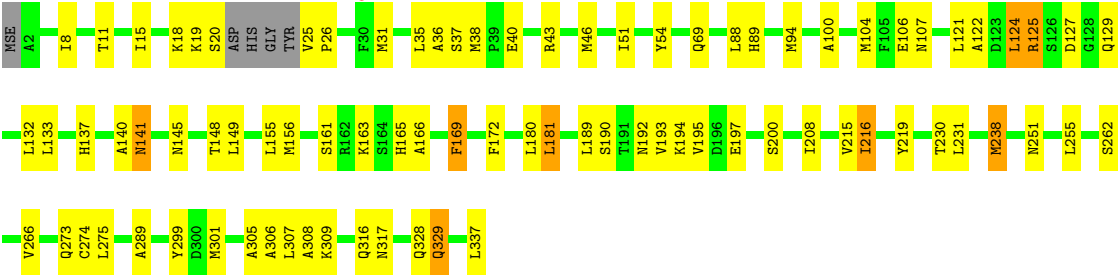
● Molecule 1: L-asparaginase I

Chain D: 

73%

23%

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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	2740 reflections (5.39%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.1	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 18.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.029 for -h,l,k 0.037 for -h,-l,-k 0.075 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10702	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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 16.

All (329) 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: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	Interatomic distance (Å)	Clash overlap (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:12:GLY:HA2	1:C:57:LEU:HD22	1.68	0.73
1:C:75:ILE:CD1	1:C:87:ILE:HD11	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ILE:CD1	1:B:254:LEU:HD11	2.23	0.69
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:C:27:VAL:HG11	1:C:57:LEU:HD12	1.75	0.68
1:D:19:LYS:HZ2	1:D:25:VAL:HG23	1.56	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:B:255:LEU:HD21	1:B:289:ALA:HB1	1.77	0.67
1:D:156:MSE:HE1	1:D:172:PHE:HB2	1.77	0.67
1:B:267:ILE:HD13	1:B:323:VAL:HG12	1.77	0.66
1:B:278:LYS:NZ	1:B:337:LEU:HD23	2.11	0.66
1:C:104:MSE:CG	1:C:208:ILE:HD12	2.25	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:245:VAL:O	1:B:245:VAL:HG12	1.98	0.63
1:B:267:ILE:HD13	1:B:323:VAL:HG11	1.80	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:A:35:LEU:HD11	1:A:122:ALA:HB2	1.80	0.62
1:B:35:LEU:HD21	1:B:122:ALA:HB2	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:163:LYS:HE2	1:A:166:ALA:HB2	1.85	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:C:183:ALA:HA	1:C:187:ILE:HD13	1.86	0.58
1:D:163:LYS:HZ2	1:D:166:ALA:HB2	1.68	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:A:316:GLN:HG3	4:A:684:HOH:O	2.05	0.56
1:B:185:ILE:CG2	1:D:169:PHE:CD1	2.89	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:B:64:THR:HG22	1:B:66:ALA:N	2.20	0.56
1:C:38:MSE:CE	1:C:129:GLN:NE2	2.68	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:C:41:PHE:CE1	1:C:133:LEU:HD13	2.41	0.56
1:D:148:THR:OG1	1:D:155:LEU:HD11	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:141:ASN:ND2	1:D:141:ASN:N	2.55	0.55
1:D:35:LEU:O	1:D:37:SER:N	2.40	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:B:129:GLN:O	1:B:133:LEU:HB2	2.09	0.53
1:D:181:LEU:HD23	1:D:181:LEU:C	2.29	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:A:34:GLN:NE2	4:A:710:HOH:O	2.42	0.51
1:C:35:LEU:O	1:C:37[A]:SER:N	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:33:LYS:HB2	1:A:33:LYS:HZ3	1.78	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: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:C:166:ALA:HB2	1:D:274:CYS:SG	2.54	0.48
1:D:35:LEU:C	1:D:37:SER:H	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:GLU:O	1:A:203:PHE:HA	2.15	0.46
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:C:255:LEU:HD11	1:C:289:ALA:HB1	1.96	0.46
1:A:30:PHE:HB3	4:A:709:HOH:O	2.15	0.46
1:C:309:LYS:CD	1:C:327:MSE:HE2	2.46	0.46
1:B:134:ASN:OD1	1:D:125:ARG:HD2	2.16	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:A:229:ASN:O	1:B:229:ASN:HB3	2.16	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:C:149:LEU:C	1:C:149:LEU:HD23	2.37	0.46
1:D:18:LYS:O	1:D:26:PRO:HD2	2.15	0.46
1:A:216:ILE:HG22	1:A:218:MSE:HE3	1.97	0.46
1:D:25:VAL:N	1:D:26:PRO:HD3	2.31	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:B:312:TYR:O	1:B:316:GLN:NE2	2.49	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: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:B:250:GLN:CG	1:B:250:GLN:O	2.62	0.44
1:C:313:LEU:CD1	1:C:327:MSE:HE3	2.34	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:B:181:LEU:HD12	1:B:181:LEU:C	2.38	0.44
1:C:38:MSE:HE2	1:C:129:GLN:NE2	2.32	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:B:129:GLN:HG3	1:B:130:ALA:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:VAL:CB	1:B:26:PRO:HD3	2.48	0.43
1:C:309:LYS:CD	1:C:327:MSE:CE	2.96	0.43
1:D:20:SER:N	1:D:25:VAL:N	2.65	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
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:A:302:THR:HG23	4:A:604:HOH:O	2.18	0.43
1:B:129:GLN:HE21	1:B:129:GLN:HB2	1.69	0.43
1:D:208:ILE:O	1:D:208:ILE:HG23	2.18	0.43
1:D:316:GLN:NE2	4:D:620:HOH:O	2.51	0.43
1:A:27:VAL:HG11	1:A:57:LEU:CD2	2.49	0.43
1:C:214:GLY:HA3	1:C:238:MSE:HE1	2.01	0.43
1:A:20:SER:OG	1:A:21:ASP:N	2.51	0.43
1:A:125:ARG:NH2	1:C:184:GLY:O	2.39	0.43
1:B:278:LYS:NZ	1:B:337:LEU:CG	2.82	0.43
1:D:11:THR:HG22	1:D:54:TYR:CE2	2.54	0.43
1:D:8:ILE:CG2	1:D:51:ILE:HD12	2.49	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:A:281:MSE:HE3	1:A:290:LEU:HB2	2.01	0.42
1:D:149:LEU:HD22	1:D:156:MSE:HE3	2.00	0.42
1:A:118:GLN:NE2	4:A:614:HOH:O	2.51	0.42
1:C:216:ILE:C	1:C:216:ILE:HD12	2.39	0.42
1:C:228:ARG:NH2	1:C:229:ASN:OD1	2.53	0.42
1:C:275:LEU:HD22	1:D:275:LEU:HD22	2.00	0.42
1:B:14:THR:HG23	1:B:17:MSE:HE2	2.01	0.42
1:B:16:GLY:HA3	1:B:32:GLU:HG2	2.00	0.42
1:C:208:ILE:O	1:C:208:ILE:HG22	2.19	0.42
1:D:40:GLU:HG3	1:D:133:LEU:HD11	2.00	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:C:238:MSE:HG3	1:C:268:VAL:HG13	2.01	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:A:231:LEU:HD21	1:A:238:MSE:HG3	2.01	0.42
1:B:94:MSE:HE2	1:B:149:LEU:HD21	2.00	0.42
1:C:327:MSE:HA	1:C:327:MSE:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:SER:HA	1:D:266:VAL:O	2.20	0.42
1:A:156:MSE:HE1	1:A:172:PHE:HB2	2.02	0.41
1:C:133:LEU:HD12	1:C:133:LEU:HA	1.95	0.41
1:A:335:MSE:HE3	1:A:337:LEU:HD21	2.01	0.41
1:C:185:ILE:HG23	1:C:186:ASN:ND2	2.34	0.41
1:C:228:ARG:CZ	1:C:228:ARG:HB3	2.51	0.41
1:C:76:ALA:HB2	1:C:205:VAL:HG21	2.02	0.41
1:B:233:GLN:NE2	4:B:677:HOH:O	2.52	0.41
1:C:117:SER:OG	1:C:119:ILE:O	2.30	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: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:C:309:LYS:HE2	1:C:327:MSE:HA	2.02	0.41
1:A:169:PHE:N	1:A:169:PHE:CD1	2.89	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:69:GLN:HA	1:D:104:MSE:HE1	2.02	0.41
1:C:214:GLY:HA3	1:C:238:MSE:HE2	2.03	0.41
1:D:124:LEU:O	1:D:124:LEU:HD23	2.21	0.41
1:B:154:ARG:CG	1:B:156:MSE:HE2	2.48	0.41
1:C:309:LYS:CE	1:C:327: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:B:31:MSE:O	1:B:35:LEU:HD13	2.22	0.40
1:C:216:ILE:CD1	1:C:240:LEU:HD23	2.47	0.40
1:A:155:LEU:HB3	1:A:181:LEU:HB3	2.03	0.40
1:C:10:TYR:CZ	1:C:16:GLY:HA3	2.55	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:143:PRO:HD2	1:C:195:VAL:CG1	2.51	0.40
1:C:309:LYS:CG	1:C:327:MSE:HE2	2.39	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%)	15	15
1	B	334/337 (99%)	312 (93%)	19 (6%)	3 (1%)	20	23
1	C	321/337 (95%)	303 (94%)	15 (5%)	3 (1%)	20	23
1	D	330/337 (98%)	311 (94%)	17 (5%)	2 (1%)	28	34
All	All	1308/1348 (97%)	1236 (94%)	60 (5%)	12 (1%)	22	23

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%)	16	21
1	B	280/262 (107%)	259 (92%)	21 (8%)	16	20
1	C	273/262 (104%)	258 (94%)	15 (6%)	25	33
1	D	276/262 (105%)	262 (95%)	14 (5%)	28	37
All	All	1102/1048 (105%)	1032 (94%)	70 (6%)	21	27

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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



## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	2.75	1 (100%)	0,3,3	0.00	-
2	ACT	B	602	-	1,3,3	2.06	1 (100%)	0,3,3	0.00	-
2	ACT	B	603	-	1,3,3	2.21	1 (100%)	0,3,3	0.00	-
2	ACT	C	604	-	1,3,3	2.88	1 (100%)	0,3,3	0.00	-
3	GOL	D	605	-	5,5,5	0.38	0	5,5,5	0.36	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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	ACT	CH3-C	2.06	1.51	1.48
2	B	603	ACT	CH3-C	2.21	1.51	1.48
2	A	601	ACT	CH3-C	2.75	1.52	1.48
2	C	604	ACT	CH3-C	2.88	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.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	ACT	3	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	313/337 (92%)	-0.76	2 (0%) 89 90	5, 15, 32, 41	2 (0%)
1	B	318/337 (94%)	-0.74	1 (0%) 93 95	9, 18, 34, 42	2 (0%)
1	C	313/337 (92%)	-0.75	1 (0%) 93 95	6, 16, 32, 56	1 (0%)
1	D	317/337 (94%)	-0.73	1 (0%) 93 95	7, 18, 36, 41	0
All	All	1261/1348 (93%)	-0.75	5 (0%) 92 93	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	B	169	PHE	2.5
1	A	192	ASN	2.5
1	A	168	GLY	2.4
1	C	30	PHE	2.2

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	GOL	D	605	6/6	0.84	0.22	8.02	63,64,64,65	0
2	ACT	C	604	4/4	0.88	0.15	2.71	47,48,49,49	0
2	ACT	A	601	4/4	0.93	0.14	1.14	37,38,38,39	0
2	ACT	B	603	4/4	0.89	0.10	0.35	51,51,51,51	0
2	ACT	B	602	4/4	0.84	0.16	-	54,54,54,54	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.