Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 08:51 am BST

PDB ID	:	3NA8
Title	:	Crystal Structure of a putative dihydrodipicolinate synthetase from Pseudomonas aeruginosa
Authors	:	Qiu, W.; Lam, R.; Romanov, V.; Jones, K.; Pai, E.F.; Chirgadze, N.Y.
Deposited on	:	2010-06-01
Resolution	:	1.85 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 following versions of software and data (see references ①) were used in the production of this report:

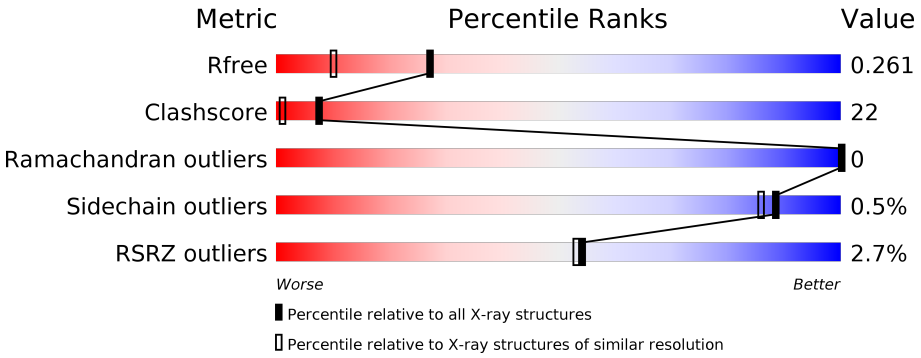
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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}	130704	2469 (1.86-1.86)
Clashscore	141614	2625 (1.86-1.86)
Ramachandran outliers	138981	2592 (1.86-1.86)
Sidechain outliers	138945	2592 (1.86-1.86)
RSRZ outliers	127900	2436 (1.86-1.86)

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 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 <=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	315	2% 67% 24% • 8%
1	B	315	% 72% 19% • 8%
1	C	315	4% 66% 26% 8%
1	D	315	3% 63% 30% 8%

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
3	MLT	D	317	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9849 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 putative dihydrodipicolinate synthetase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	291	Total	C	N	O	S	Se	0	5	0
			2249	1434	392	415	3	5			
1	B	290	Total	C	N	O	S	Se	3	7	0
			2255	1438	394	415	3	5			
1	C	291	Total	C	N	O	S	Se	0	2	0
			2224	1421	382	412	3	6			
1	D	290	Total	C	N	O	S	Se	5	8	0
			2261	1444	394	414	3	6			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP Q9I6R5
A	2	GLY	-	expression tag	UNP Q9I6R5
A	3	SER	-	expression tag	UNP Q9I6R5
A	4	SER	-	expression tag	UNP Q9I6R5
A	5	HIS	-	expression tag	UNP Q9I6R5
A	6	HIS	-	expression tag	UNP Q9I6R5
A	7	HIS	-	expression tag	UNP Q9I6R5
A	8	HIS	-	expression tag	UNP Q9I6R5
A	9	HIS	-	expression tag	UNP Q9I6R5
A	10	HIS	-	expression tag	UNP Q9I6R5
A	11	SER	-	expression tag	UNP Q9I6R5
A	12	SER	-	expression tag	UNP Q9I6R5
A	13	GLY	-	expression tag	UNP Q9I6R5
A	14	LEU	-	expression tag	UNP Q9I6R5
A	15	VAL	-	expression tag	UNP Q9I6R5
A	16	PRO	-	expression tag	UNP Q9I6R5
A	17	ARG	-	expression tag	UNP Q9I6R5
A	18	GLY	-	expression tag	UNP Q9I6R5
A	19	SER	-	expression tag	UNP Q9I6R5
A	20	HIS	-	expression tag	UNP Q9I6R5
A	314	GLY	-	expression tag	UNP Q9I6R5

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Chain	Residue	Modelled	Actual	Comment	Reference
A	315	SER	-	expression tag	UNP Q9I6R5
B	1	MSE	-	expression tag	UNP Q9I6R5
B	2	GLY	-	expression tag	UNP Q9I6R5
B	3	SER	-	expression tag	UNP Q9I6R5
B	4	SER	-	expression tag	UNP Q9I6R5
B	5	HIS	-	expression tag	UNP Q9I6R5
B	6	HIS	-	expression tag	UNP Q9I6R5
B	7	HIS	-	expression tag	UNP Q9I6R5
B	8	HIS	-	expression tag	UNP Q9I6R5
B	9	HIS	-	expression tag	UNP Q9I6R5
B	10	HIS	-	expression tag	UNP Q9I6R5
B	11	SER	-	expression tag	UNP Q9I6R5
B	12	SER	-	expression tag	UNP Q9I6R5
B	13	GLY	-	expression tag	UNP Q9I6R5
B	14	LEU	-	expression tag	UNP Q9I6R5
B	15	VAL	-	expression tag	UNP Q9I6R5
B	16	PRO	-	expression tag	UNP Q9I6R5
B	17	ARG	-	expression tag	UNP Q9I6R5
B	18	GLY	-	expression tag	UNP Q9I6R5
B	19	SER	-	expression tag	UNP Q9I6R5
B	20	HIS	-	expression tag	UNP Q9I6R5
B	314	GLY	-	expression tag	UNP Q9I6R5
B	315	SER	-	expression tag	UNP Q9I6R5
C	1	MSE	-	expression tag	UNP Q9I6R5
C	2	GLY	-	expression tag	UNP Q9I6R5
C	3	SER	-	expression tag	UNP Q9I6R5
C	4	SER	-	expression tag	UNP Q9I6R5
C	5	HIS	-	expression tag	UNP Q9I6R5
C	6	HIS	-	expression tag	UNP Q9I6R5
C	7	HIS	-	expression tag	UNP Q9I6R5
C	8	HIS	-	expression tag	UNP Q9I6R5
C	9	HIS	-	expression tag	UNP Q9I6R5
C	10	HIS	-	expression tag	UNP Q9I6R5
C	11	SER	-	expression tag	UNP Q9I6R5
C	12	SER	-	expression tag	UNP Q9I6R5
C	13	GLY	-	expression tag	UNP Q9I6R5
C	14	LEU	-	expression tag	UNP Q9I6R5
C	15	VAL	-	expression tag	UNP Q9I6R5
C	16	PRO	-	expression tag	UNP Q9I6R5
C	17	ARG	-	expression tag	UNP Q9I6R5
C	18	GLY	-	expression tag	UNP Q9I6R5
C	19	SER	-	expression tag	UNP Q9I6R5

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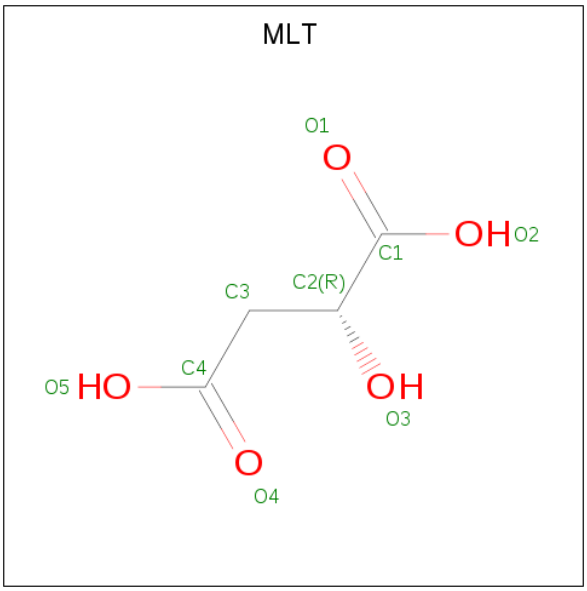
Chain	Residue	Modelled	Actual	Comment	Reference
C	20	HIS	-	expression tag	UNP Q9I6R5
C	314	GLY	-	expression tag	UNP Q9I6R5
C	315	SER	-	expression tag	UNP Q9I6R5
D	1	MSE	-	expression tag	UNP Q9I6R5
D	2	GLY	-	expression tag	UNP Q9I6R5
D	3	SER	-	expression tag	UNP Q9I6R5
D	4	SER	-	expression tag	UNP Q9I6R5
D	5	HIS	-	expression tag	UNP Q9I6R5
D	6	HIS	-	expression tag	UNP Q9I6R5
D	7	HIS	-	expression tag	UNP Q9I6R5
D	8	HIS	-	expression tag	UNP Q9I6R5
D	9	HIS	-	expression tag	UNP Q9I6R5
D	10	HIS	-	expression tag	UNP Q9I6R5
D	11	SER	-	expression tag	UNP Q9I6R5
D	12	SER	-	expression tag	UNP Q9I6R5
D	13	GLY	-	expression tag	UNP Q9I6R5
D	14	LEU	-	expression tag	UNP Q9I6R5
D	15	VAL	-	expression tag	UNP Q9I6R5
D	16	PRO	-	expression tag	UNP Q9I6R5
D	17	ARG	-	expression tag	UNP Q9I6R5
D	18	GLY	-	expression tag	UNP Q9I6R5
D	19	SER	-	expression tag	UNP Q9I6R5
D	20	HIS	-	expression tag	UNP Q9I6R5
D	314	GLY	-	expression tag	UNP Q9I6R5
D	315	SER	-	expression tag	UNP Q9I6R5

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

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

- Molecule 3 is D-MALATE (three-letter code: MLT) (formula: $C_4H_6O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 9 4 5	0	0
3	C	1	Total C O 9 4 5	0	0
3	D	1	Total C O 9 4 5	0	0

- Molecule 4 is water.

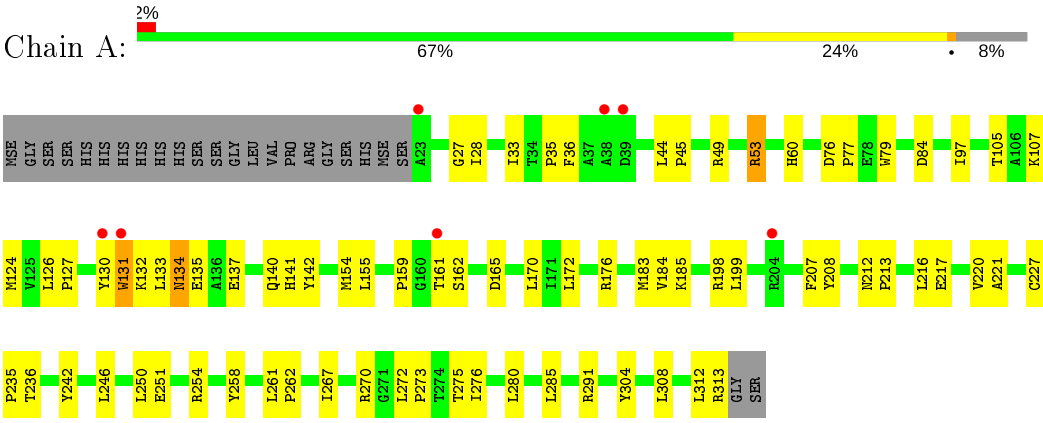
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	258	Total O 258 258	0	0
4	B	248	Total O 248 248	0	0
4	C	166	Total O 166 166	0	0
4	D	157	Total O 157 157	0	0

3 Residue-property plots (i)

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.

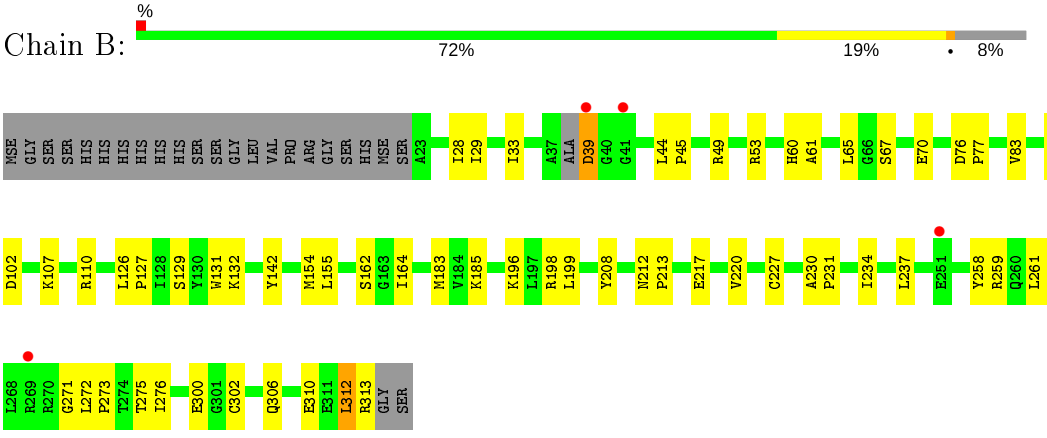
- Molecule 1: putative dihydrodipicolinate synthetase

Chain A:



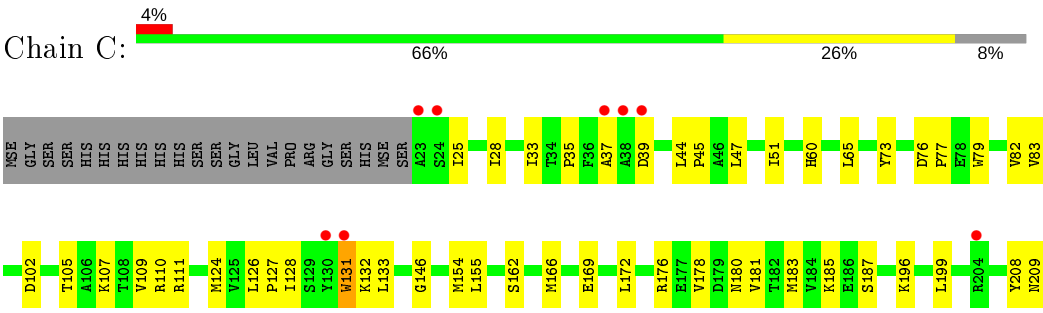
- Molecule 1: putative dihydrodipicolinate synthetase

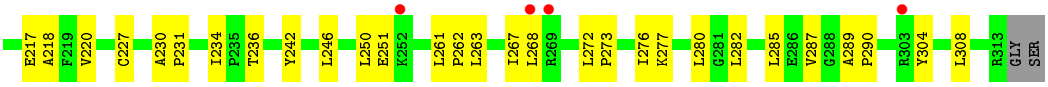
Chain B:



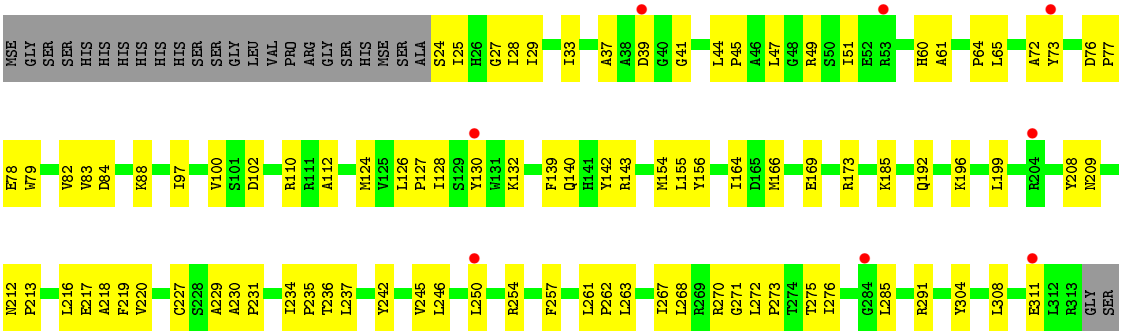
- Molecule 1: putative dihydrodipicolinate synthetase

Chain C:





- Molecule 1: putative dihydrodipicolinate synthetase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	107.37Å 156.21Å 76.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.06 – 1.85 43.06 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.3 (43.06-1.85) 96.3 (43.06-1.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.19 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.235 , 0.270 0.228 , 0.261	Depositor DCC
R_{free} test set	5334 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	27.3	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9849	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, CSO, MLT

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	0.34	0/2294	0.41	0/3108
1	B	0.35	0/2306	0.44	3/3121 (0.1%)
1	C	0.20	0/2260	0.36	0/3064
1	D	0.22	0/2315	0.36	0/3135
All	All	0.29	0/9175	0.39	3/12428 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	312	LEU	CB-CG-CD2	-6.17	100.50	111.00
1	B	313	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	B	313	ARG	NE-CZ-NH2	5.70	123.15	120.30

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	2249	0	2298	98	0
1	B	2255	0	2308	74	0
1	C	2224	0	2267	118	0
1	D	2261	0	2324	137	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	9	0	4	1	0
3	C	9	0	4	2	0
3	D	9	0	4	16	0
4	A	258	0	0	16	0
4	B	248	0	0	5	0
4	C	166	0	0	15	0
4	D	157	0	0	9	0
All	All	9849	0	9209	400	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 22.

All (400) 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:D:237:LEU:N	3:D:317:MLT:O5	1.75	1.19
1:B:185:LYS:NZ	1:B:227:CYS:SG	2.17	1.18
1:A:251:GLU:HG2	4:A:420:HOH:O	1.44	1.17
1:B:300:GLU:HB2	4:B:752:HOH:O	1.46	1.12
1:D:236:THR:H	3:D:317:MLT:H31	0.97	1.09
1:D:185:LYS:NZ	1:D:227:CYS:SG	2.26	1.08
1:D:124:MSE:SE	1:D:154[A]:MSE:HE3	2.05	1.05
1:A:53:ARG:HD2	4:A:414:HOH:O	1.56	1.04
1:B:70:GLU:HA	1:C:131:TRP:HH2	1.21	1.02
1:A:250:LEU:HD21	1:A:254[B]:ARG:HH12	1.25	1.01
1:A:124:MSE:HG3	1:A:154:MSE:HG2	1.39	1.00
1:D:236:THR:H	3:D:317:MLT:C3	1.75	0.99
1:A:154:MSE:HE1	1:A:208:TYR:CD2	1.98	0.98
1:D:236:THR:N	3:D:317:MLT:H31	1.77	0.97
1:B:272:LEU:HB2	1:B:273:PRO:HD3	1.49	0.95
1:B:28:ILE:H	1:B:60:HIS:HD2	1.15	0.94
1:A:28:ILE:H	1:A:60:HIS:HD2	1.16	0.93
1:C:304:TYR:CE2	1:C:308:LEU:HD11	2.04	0.92
1:D:97:ILE:CD1	1:D:154[A]:MSE:HE2	2.00	0.92
1:D:236:THR:HB	3:D:317:MLT:C4	1.99	0.92
1:A:217:GLU:O	1:A:220:VAL:HG22	1.70	0.91
1:B:237:LEU:HD21	1:B:259[B]:ARG:NH1	1.85	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:ILE:H	1:C:60:HIS:HD2	1.12	0.90
1:B:154:MSE:HE1	1:B:208:TYR:CD2	2.08	0.89
1:D:97:ILE:HD13	1:D:154[A]:MSE:HE2	1.54	0.89
1:D:304:TYR:CE2	1:D:308:LEU:HD11	2.09	0.88
1:A:250:LEU:CD2	1:A:254[B]:ARG:HH12	1.87	0.87
1:C:176:ARG:HD2	4:C:412:HOH:O	1.73	0.87
1:A:185:LYS:NZ	1:A:227:CYS:SG	2.48	0.87
1:B:67:SER:O	1:C:131:TRP:CZ3	2.29	0.85
1:D:28:ILE:H	1:D:60:HIS:HD2	1.22	0.85
1:D:304:TYR:HE2	1:D:308:LEU:HD11	1.42	0.83
1:B:67:SER:O	1:C:131:TRP:HZ3	1.62	0.82
1:C:251:GLU:HG3	4:C:382:HOH:O	1.79	0.82
1:D:140[A]:GLN:HG2	4:D:957:HOH:O	1.79	0.82
1:C:154[B]:MSE:HE1	1:C:208:TYR:CD2	2.14	0.82
1:D:24:SER:HA	4:D:942:HOH:O	1.79	0.82
1:D:268:LEU:HD13	1:D:268:LEU:O	1.79	0.81
1:D:124:MSE:HE2	1:D:154[A]:MSE:CE	2.10	0.80
1:C:234:ILE:HD13	1:C:263:LEU:HD23	1.62	0.80
1:D:267:ILE:CG2	1:D:272:LEU:HD23	2.12	0.80
1:C:28:ILE:H	1:C:60:HIS:CD2	1.98	0.80
1:A:134:ASN:ND2	1:A:137:GLU:H	1.79	0.79
1:C:185:LYS:NZ	1:C:227:CYS:SG	2.53	0.79
1:A:131:TRP:HZ2	1:D:272:LEU:HG	1.46	0.79
1:B:70:GLU:HA	1:C:131:TRP:CH2	2.14	0.78
1:B:28:ILE:H	1:B:60:HIS:CD2	1.99	0.78
1:D:192:GLN:O	1:D:196:LYS:HG3	1.85	0.77
1:A:250:LEU:HD21	1:A:254[B]:ARG:NH1	2.00	0.76
1:D:37:ALA:HB3	1:D:39[B]:ASP:OD1	1.85	0.76
1:C:217:GLU:O	1:C:220:VAL:HG22	1.85	0.76
1:D:102:ASP:HA	1:D:128:ILE:HD11	1.69	0.75
1:A:161:THR:HG21	4:A:456:HOH:O	1.85	0.75
1:D:97:ILE:HD13	1:D:154[A]:MSE:CE	2.16	0.75
1:A:132:LYS:HG3	1:A:133:LEU:N	2.01	0.74
1:C:124:MSE:HG3	1:C:154[B]:MSE:HG2	1.68	0.74
1:C:304:TYR:HE2	1:C:308:LEU:HD11	1.49	0.73
1:C:107:LYS:HG2	1:C:111:ARG:HD2	1.70	0.73
1:C:126:LEU:HD12	1:C:127:PRO:HD2	1.71	0.72
1:D:102:ASP:CA	1:D:128:ILE:HD11	2.20	0.71
1:D:268:LEU:HD13	1:D:268:LEU:C	2.11	0.71
1:D:250:LEU:HD13	1:D:250:LEU:O	1.90	0.71
1:A:216:LEU:O	1:A:220:VAL:HG13	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:196:LYS:HE3	4:B:546:HOH:O	1.90	0.71
1:D:235:PRO:HD2	3:D:317:MLT:H32	1.73	0.71
1:D:28:ILE:H	1:D:60:HIS:CD2	2.08	0.71
1:A:28:ILE:H	1:A:60:HIS:CD2	2.06	0.70
1:D:250:LEU:HD13	1:D:250:LEU:C	2.11	0.70
1:A:154:MSE:CE	1:A:208:TYR:CD2	2.75	0.70
1:C:110:ARG:HD3	1:C:110:ARG:C	2.11	0.70
1:A:172:LEU:O	1:A:176:ARG:HG3	1.90	0.69
1:A:134:ASN:HD22	1:A:134:ASN:C	1.95	0.69
1:C:217:GLU:O	1:C:220:VAL:CG2	2.41	0.69
1:B:102:ASP:OD1	1:B:107:LYS:HD3	1.91	0.69
1:C:172:LEU:O	1:C:176:ARG:HG3	1.93	0.69
1:D:60:HIS:HE1	4:D:958:HOH:O	1.76	0.68
1:D:236:THR:HB	3:D:317:MLT:C3	2.23	0.68
1:A:161:THR:HG23	1:D:130:TYR:O	1.94	0.68
1:A:60:HIS:HE1	4:A:659:HOH:O	1.76	0.67
1:D:230:ALA:N	1:D:231:PRO:CD	2.56	0.67
1:D:97:ILE:HD11	1:D:154[A]:MSE:HE2	1.75	0.67
1:C:272:LEU:HB2	1:C:273:PRO:CD	2.24	0.66
1:D:110:ARG:C	1:D:110:ARG:HD3	2.15	0.66
1:B:154:MSE:SE	1:B:185:LYS:HE2	2.46	0.66
1:B:67:SER:CA	1:C:131:TRP:HZ3	2.08	0.65
1:C:242:TYR:CE2	1:C:246:LEU:HD11	2.31	0.65
1:A:199:LEU:HD11	1:B:261:LEU:HD23	1.78	0.65
1:A:254[B]:ARG:HD3	1:B:220:VAL:O	1.96	0.65
1:D:65:LEU:HD13	1:D:79:TRP:NE1	2.12	0.65
1:B:126:LEU:HD12	1:B:127:PRO:HD2	1.77	0.64
1:D:154[B]:MSE:SE	1:D:185:LYS:HE2	2.47	0.64
1:B:272:LEU:CB	1:B:273:PRO:HD3	2.23	0.64
1:D:124:MSE:HE2	1:D:154[A]:MSE:HE1	1.78	0.64
1:A:230:ALA:N	1:A:231:PRO:CD	2.61	0.63
1:C:250:LEU:C	1:C:250:LEU:HD23	2.18	0.63
1:C:154[B]:MSE:CE	1:C:208:TYR:CD2	2.82	0.63
1:D:124:MSE:HG3	1:D:154[B]:MSE:HG2	1.81	0.63
1:A:251:GLU:CG	4:A:420:HOH:O	2.20	0.63
1:D:124:MSE:CG	1:D:154[A]:MSE:HE3	2.29	0.63
1:D:49[B]:ARG:NH1	1:D:285:LEU:HD12	2.14	0.62
1:A:236:THR:OG1	3:A:317:MLT:O5	2.16	0.62
1:B:154:MSE:CE	1:B:208:TYR:CD2	2.81	0.62
1:D:84:ASP:OD1	1:D:88:LYS:HE3	2.00	0.62
1:D:97:ILE:O	1:D:97:ILE:HG23	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:ASN:HB2	1:C:213:PRO:HD3	1.82	0.62
1:B:67:SER:C	1:C:131:TRP:HZ3	2.02	0.62
1:C:230:ALA:N	1:C:231:PRO:CD	2.63	0.61
1:C:33[B]:ILE:CD1	1:C:280:LEU:HD12	2.31	0.61
1:C:126:LEU:HD21	1:C:162:SER:HB3	1.83	0.61
1:A:250:LEU:CD2	1:A:254[B]:ARG:NH1	2.61	0.61
1:B:230:ALA:N	1:B:231:PRO:CD	2.63	0.61
1:C:199:LEU:HD11	1:D:261:LEU:HD23	1.82	0.60
1:C:33[A]:ILE:CD1	1:C:35:PRO:HD3	2.31	0.60
1:C:285:LEU:HD22	1:C:287:VAL:HG13	1.83	0.60
1:D:234:ILE:HD13	1:D:263:LEU:HD23	1.83	0.60
1:B:88:LYS:HE3	4:B:625:HOH:O	2.03	0.59
1:C:217:GLU:HA	1:C:220:VAL:HG22	1.84	0.59
1:B:217:GLU:HA	1:B:220:VAL:HG22	1.85	0.59
1:C:155:LEU:HD21	1:C:166:MSE:CE	2.33	0.59
1:C:25:ILE:HA	4:C:331:HOH:O	2.02	0.59
1:A:154:MSE:SE	1:A:185:LYS:HE2	2.53	0.59
1:B:88:LYS:CE	4:B:625:HOH:O	2.50	0.59
1:C:272:LEU:O	1:C:276:ILE:HG12	2.03	0.59
1:C:220:VAL:HG11	1:D:220[B]:VAL:HG11	1.84	0.59
1:A:140[B]:GLN:HG2	4:A:428:HOH:O	2.03	0.59
1:D:234:ILE:HA	3:D:317:MLT:H32	1.84	0.58
1:D:185:LYS:HZ1	1:D:227:CYS:CB	2.15	0.58
1:D:272:LEU:HB2	1:D:273:PRO:CD	2.33	0.58
1:C:217:GLU:C	1:C:220:VAL:HG22	2.24	0.58
1:A:250:LEU:HD23	1:A:250:LEU:C	2.24	0.58
1:B:110:ARG:HD3	1:B:110:ARG:C	2.23	0.58
1:C:217:GLU:HA	1:C:220:VAL:CG2	2.34	0.58
1:D:37:ALA:CB	1:D:39[B]:ASP:OD1	2.52	0.58
1:A:272:LEU:HB2	1:A:273:PRO:CD	2.34	0.57
1:D:124:MSE:CE	1:D:154[A]:MSE:CE	2.80	0.57
1:D:29:ILE:HD12	1:D:29:ILE:N	2.19	0.57
1:D:235:PRO:CD	3:D:317:MLT:H32	2.35	0.57
1:C:33[A]:ILE:HD12	1:C:35:PRO:HD3	1.87	0.57
1:D:311:GLU:HB2	4:D:987:HOH:O	2.04	0.56
1:D:270:ARG:HB2	1:D:275:THR:CG2	2.35	0.56
1:C:154[A]:MSE:SE	1:C:185:LYS:HE2	2.56	0.56
1:D:124:MSE:SE	1:D:154[A]:MSE:CE	2.93	0.56
1:D:140[A]:GLN:HE22	1:D:143:ARG:HD3	1.71	0.56
1:C:33[B]:ILE:HD13	1:C:280:LEU:HD12	1.87	0.56
1:A:53:ARG:HH11	1:A:280:LEU:HD23	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ILE:CD1	1:A:35:PRO:HG3	2.36	0.56
1:C:176:ARG:CG	4:C:498:HOH:O	2.54	0.56
1:A:212:ASN:HB2	4:A:408:HOH:O	2.06	0.56
1:A:304:TYR:CE2	1:A:308:LEU:HD11	2.41	0.56
1:B:272:LEU:HB2	1:B:273:PRO:CD	2.31	0.56
1:B:33:ILE:O	1:B:33:ILE:HD12	2.06	0.56
1:B:76:ASP:HB2	1:B:77:PRO:HD3	1.88	0.56
1:A:217:GLU:C	1:A:220:VAL:HG22	2.25	0.56
1:D:33:ILE:HD12	1:D:33:ILE:C	2.26	0.55
1:B:33:ILE:C	1:B:33:ILE:HD12	2.26	0.55
1:A:97:ILE:HG23	1:A:97:ILE:O	2.07	0.55
1:D:236:THR:CB	3:D:317:MLT:H31	2.37	0.55
1:C:272:LEU:HB2	1:C:273:PRO:HD3	1.89	0.55
1:A:217:GLU:O	1:A:220:VAL:CG2	2.50	0.55
1:D:155:LEU:C	1:D:155:LEU:HD23	2.27	0.55
1:B:154:MSE:HE1	1:B:208:TYR:CG	2.41	0.55
1:D:65:LEU:HD13	1:D:79:TRP:CE2	2.42	0.55
1:A:134:ASN:HD21	1:A:137:GLU:H	1.53	0.54
1:C:97:ILE:O	1:C:97:ILE:HG23	2.08	0.54
1:A:49:ARG:HD2	4:A:554:HOH:O	2.06	0.54
1:A:127:PRO:HD3	1:A:142:TYR:OH	2.07	0.54
1:A:97:ILE:HD11	1:A:154:MSE:HB3	1.89	0.54
1:C:97:ILE:HD11	1:C:154[B]:MSE:HB3	1.90	0.54
1:C:251:GLU:CG	4:C:382:HOH:O	2.48	0.54
1:A:126:LEU:HD11	1:A:162:SER:HB3	1.88	0.54
1:C:88:LYS:HG3	4:C:906:HOH:O	2.07	0.54
1:A:185:LYS:HZ1	1:A:227:CYS:HG	1.52	0.54
4:A:1002:HOH:O	1:D:140[B]:GLN:HG2	2.08	0.54
1:A:130:TYR:HA	4:D:779:HOH:O	2.08	0.54
1:C:261:LEU:HB3	1:C:262:PRO:HD3	1.90	0.53
1:C:272:LEU:CB	1:C:273:PRO:CD	2.87	0.53
1:A:242:TYR:CE2	1:A:246:LEU:HD11	2.44	0.53
1:A:36:PHE:CE2	1:A:291:ARG:HG3	2.44	0.53
1:B:185:LYS:CE	1:B:227:CYS:SG	2.97	0.53
1:A:107:LYS:HG3	1:A:110:ARG:NH2	2.24	0.53
1:C:65:LEU:HD13	1:C:79:TRP:NE1	2.24	0.52
1:D:139:PHE:CD1	1:D:173[B]:ARG:NH2	2.76	0.52
1:C:102:ASP:HA	1:C:128:ILE:HD11	1.91	0.52
1:D:267:ILE:HG22	1:D:272:LEU:HD23	1.89	0.52
1:A:131:TRP:HZ2	1:D:272:LEU:CG	2.17	0.52
1:B:126:LEU:HD21	1:B:162:SER:HB3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:ILE:HG13	1:D:61:ALA:HB3	1.91	0.52
1:B:39:ASP:CG	1:B:39:ASP:O	2.48	0.52
1:D:185:LYS:NZ	1:D:227:CYS:CB	2.71	0.52
1:D:33:ILE:HD12	1:D:33:ILE:O	2.10	0.52
1:A:267:ILE:CG2	1:A:272:LEU:HD23	2.40	0.52
1:B:127:PRO:HD3	1:B:142:TYR:OH	2.09	0.52
1:D:124:MSE:HG3	1:D:154[A]:MSE:HE3	1.90	0.52
1:D:76:ASP:HB2	1:D:77:PRO:HD3	1.90	0.52
1:A:33:ILE:HD12	1:A:35:PRO:HD3	1.92	0.52
1:A:53:ARG:CD	4:A:414:HOH:O	2.31	0.52
1:B:217:GLU:O	1:B:220:VAL:HG22	2.09	0.52
1:C:217:GLU:CA	1:C:220:VAL:HG22	2.39	0.52
1:A:217:GLU:HA	1:A:220:VAL:HG22	1.91	0.52
1:A:313:ARG:C	4:A:542:HOH:O	2.47	0.52
1:D:236:THR:HB	3:D:317:MLT:O5	2.08	0.52
1:A:107:LYS:HG2	1:A:111[B]:ARG:HD2	1.91	0.52
1:B:129:SER:OG	1:B:131:TRP:O	2.24	0.52
1:C:169:GLU:OE2	1:C:196:LYS:NZ	2.31	0.51
1:B:97:ILE:HD11	1:B:154:MSE:HB3	1.92	0.51
1:C:251:GLU:CB	4:C:382:HOH:O	2.58	0.51
1:A:231:PRO:O	1:A:235:PRO:HD3	2.10	0.51
1:A:76:ASP:HB2	1:A:77:PRO:HD3	1.93	0.51
1:D:126:LEU:HD12	1:D:127:PRO:HD2	1.93	0.51
1:B:102:ASP:OD1	1:B:107:LYS:CD	2.59	0.51
1:B:67:SER:HA	1:C:131:TRP:HZ3	1.75	0.51
1:A:53:ARG:CZ	4:A:427:HOH:O	2.58	0.51
1:B:234:ILE:HD13	1:B:263:LEU:HD23	1.92	0.51
1:C:37:ALA:HB3	1:C:39:ASP:OD1	2.11	0.51
1:C:250:LEU:HD23	1:C:250:LEU:O	2.10	0.50
1:D:217:GLU:O	1:D:220[A]:VAL:HG22	2.11	0.50
1:D:304:TYR:CE2	1:D:308:LEU:CD1	2.88	0.50
1:D:140[A]:GLN:HE22	1:D:143:ARG:HH11	1.58	0.50
1:D:217:GLU:HA	1:D:220[A]:VAL:HG22	1.94	0.50
1:A:131:TRP:CZ2	1:D:272:LEU:HG	2.35	0.50
1:A:272:LEU:O	1:A:276:ILE:HG12	2.11	0.50
1:C:65:LEU:HD21	1:C:82:VAL:HG11	1.93	0.50
1:A:154:MSE:HE1	1:A:208:TYR:CG	2.45	0.50
1:C:176:ARG:CD	4:C:412:HOH:O	2.47	0.50
1:D:65:LEU:HD11	1:D:83:VAL:HG23	1.94	0.50
1:A:250:LEU:HD21	1:A:254[A]:ARG:NH1	2.26	0.50
1:C:155:LEU:HD21	1:C:166:MSE:HE1	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:LEU:C	1:D:250:LEU:CD1	2.79	0.50
1:B:76:ASP:N	1:B:77:PRO:CD	2.75	0.50
1:C:33[A]:ILE:HD11	1:C:35:PRO:HG3	1.94	0.50
1:D:236:THR:CB	3:D:317:MLT:C3	2.89	0.50
1:A:154:MSE:HE3	1:A:183:MSE:HB3	1.94	0.49
1:B:267:ILE:CG2	1:B:272:LEU:HD23	2.42	0.49
1:A:126:LEU:HD12	1:A:127:PRO:HD2	1.95	0.49
1:D:185:LYS:NZ	1:D:227:CYS:HB2	2.26	0.49
1:D:49[B]:ARG:CZ	1:D:285:LEU:CD1	2.91	0.49
1:C:176:ARG:HG2	4:C:505:HOH:O	2.12	0.49
1:D:268:LEU:CD1	1:D:268:LEU:C	2.80	0.49
1:D:44:LEU:N	1:D:45:PRO:CD	2.75	0.49
1:C:176:ARG:HG3	4:C:498:HOH:O	2.13	0.49
1:D:261:LEU:HB3	1:D:262:PRO:HD3	1.95	0.49
1:A:141:HIS:HE1	4:A:366:HOH:O	1.96	0.49
1:C:124:MSE:HE2	1:C:154[A]:MSE:SE	2.62	0.49
1:C:285:LEU:HD22	1:C:287:VAL:CG1	2.43	0.49
1:A:131:TRP:HE3	1:A:132:LYS:H	1.61	0.48
1:D:217:GLU:O	1:D:220[A]:VAL:CG2	2.61	0.48
1:D:236:THR:CA	3:D:317:MLT:O5	2.61	0.48
1:B:44:LEU:N	1:B:45:PRO:CD	2.76	0.48
1:C:267:ILE:CG2	1:C:272:LEU:HD23	2.43	0.48
1:C:154[B]:MSE:HE1	1:C:208:TYR:CE2	2.47	0.48
1:A:130:TYR:HE2	1:D:72:ALA:HB1	1.77	0.48
1:A:155:LEU:HD23	1:A:155:LEU:C	2.34	0.48
1:B:185:LYS:NZ	1:B:227:CYS:CB	2.76	0.48
1:C:132:LYS:HE3	1:C:133:LEU:O	2.14	0.48
1:B:261:LEU:HB3	1:B:262:PRO:HD3	1.94	0.48
1:B:49:ARG:O	1:B:53[B]:ARG:HG2	2.14	0.48
1:B:67:SER:HA	1:C:131:TRP:CZ3	2.48	0.48
1:C:187:SER:OG	1:C:210:GLY:HA3	2.13	0.48
1:C:33[A]:ILE:CD1	1:C:35:PRO:HG3	2.43	0.48
1:C:154[B]:MSE:HE3	1:C:183:MSE:HB3	1.95	0.48
1:D:216:LEU:O	1:D:220[B]:VAL:HG23	2.13	0.48
1:D:272:LEU:CB	1:D:273:PRO:CD	2.91	0.48
1:D:185:LYS:CE	1:D:227:CYS:SG	3.01	0.48
1:D:273:PRO:HG2	4:D:1047:HOH:O	2.13	0.48
1:D:65:LEU:HD12	1:D:83:VAL:HG22	1.96	0.48
1:A:134:ASN:ND2	1:A:134:ASN:C	2.65	0.47
1:A:105:THR:OG1	1:A:141:HIS:HD2	1.97	0.47
1:C:230:ALA:N	1:C:231:PRO:HD2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:SER:CA	1:C:131:TRP:CZ3	2.95	0.47
1:A:258:TYR:CZ	1:B:198[A]:ARG:HG2	2.50	0.47
1:A:84:ASP:OD1	4:A:386:HOH:O	2.20	0.47
1:B:272:LEU:CB	1:B:273:PRO:CD	2.89	0.47
1:D:25:ILE:N	4:D:942:HOH:O	2.35	0.47
1:A:130:TYR:HE2	1:D:72:ALA:CB	2.28	0.47
1:A:212:ASN:HB2	1:A:213:PRO:HD3	1.96	0.47
1:A:272:LEU:HB2	1:A:273:PRO:HD3	1.97	0.47
1:D:78:GLU:O	1:D:82:VAL:HG23	2.14	0.47
1:C:154[B]:MSE:CE	1:C:183:MSE:HB3	2.45	0.47
1:D:127:PRO:HD3	1:D:142:TYR:OH	2.15	0.47
1:D:76:ASP:N	1:D:77:PRO:CD	2.77	0.47
1:A:135:GLU:HG2	1:A:170:LEU:HD22	1.97	0.46
1:C:154[B]:MSE:SE	1:C:185:LYS:HE2	2.64	0.46
1:A:230:ALA:N	1:A:231:PRO:HD2	2.30	0.46
1:D:219:PHE:HB3	1:D:245:VAL:HG11	1.97	0.46
1:D:229:ALA:C	1:D:231:PRO:HD2	2.35	0.46
1:D:73:TYR:HD2	1:D:291:ARG:HB3	1.80	0.46
1:D:65:LEU:HD11	1:D:83:VAL:CG2	2.45	0.46
1:C:268:LEU:HB2	4:C:943:HOH:O	2.16	0.46
1:D:132:LYS:HD2	1:D:164:ILE:CD1	2.45	0.46
1:A:312:LEU:HD11	4:A:376:HOH:O	2.16	0.46
1:C:220:VAL:HG12	1:D:250:LEU:HD21	1.97	0.46
1:B:131:TRP:HZ2	1:C:73:TYR:CE2	2.34	0.46
1:D:65:LEU:CD1	1:D:83:VAL:HG22	2.46	0.46
1:D:126:LEU:HD12	1:D:156:TYR:O	2.16	0.46
1:D:65:LEU:CD1	1:D:83:VAL:CG2	2.94	0.46
1:C:65:LEU:HD13	1:C:79:TRP:CE2	2.51	0.45
1:D:100:VAL:HG11	1:D:112:ALA:HA	1.97	0.45
1:B:310:GLU:HG3	4:B:448:HOH:O	2.16	0.45
1:B:312:LEU:HA	1:B:312:LEU:HD23	1.35	0.45
1:C:146:GLY:O	1:C:180:ASN:ND2	2.47	0.45
1:D:185:LYS:HZ2	1:D:227:CYS:HB2	1.81	0.45
1:A:44:LEU:N	1:A:45:PRO:CD	2.79	0.45
1:B:155:LEU:C	1:B:155:LEU:HD23	2.36	0.45
1:C:110:ARG:HD3	1:C:110:ARG:O	2.16	0.45
1:C:33[B]:ILE:HD11	1:C:280:LEU:HD12	1.98	0.45
1:D:230:ALA:N	1:D:231:PRO:HD2	2.30	0.45
1:B:271:GLY:O	1:B:275:THR:HG23	2.17	0.45
1:B:185:LYS:HZ1	1:B:227:CYS:CB	2.17	0.45
1:C:211:CSO:SG	1:C:213:PRO:HD2	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:ASN:N	1:B:213:PRO:HD2	2.32	0.45
1:C:76:ASP:N	1:C:77:PRO:CD	2.80	0.44
1:C:209:ASN:HB2	1:C:218:ALA:HB1	1.99	0.44
1:C:282:LEU:HG	4:C:962:HOH:O	2.17	0.44
1:D:212:ASN:N	1:D:213:PRO:HD2	2.33	0.44
1:A:27:GLY:HA2	1:A:242:TYR:CE1	2.52	0.44
1:A:261:LEU:N	1:A:262:PRO:CD	2.81	0.44
1:A:33:ILE:C	1:A:33:ILE:HD12	2.38	0.44
1:C:44:LEU:N	1:C:45:PRO:CD	2.81	0.44
1:C:28:ILE:N	1:C:60:HIS:HD2	1.95	0.44
1:A:285:LEU:HD13	4:A:554:HOH:O	2.17	0.44
1:C:234:ILE:CD1	1:C:263:LEU:HD23	2.41	0.44
1:B:302:CYS:O	1:B:306:GLN:HG3	2.18	0.44
1:D:209:ASN:HB2	1:D:218:ALA:HB1	1.99	0.44
1:D:41:GLY:HA2	4:D:444:HOH:O	2.16	0.44
1:B:217:GLU:HA	1:B:220:VAL:CG2	2.48	0.43
1:A:261:LEU:HD23	1:B:199:LEU:HD11	1.99	0.43
1:A:217:GLU:CA	1:A:220:VAL:HG22	2.48	0.43
1:A:270:ARG:HB2	1:A:275:THR:CG2	2.48	0.43
1:D:169:GLU:CD	1:D:169:GLU:H	2.20	0.43
1:B:65:LEU:CD1	1:B:83:VAL:HG22	2.48	0.43
1:C:102:ASP:CA	1:C:128:ILE:HD11	2.48	0.43
1:D:236:THR:N	3:D:317:MLT:O5	2.51	0.43
1:B:154:MSE:HE3	1:B:183:MSE:HB3	2.00	0.43
1:C:285:LEU:CD2	1:C:287:VAL:HG13	2.48	0.43
1:A:272:LEU:CB	1:A:273:PRO:CD	2.95	0.43
1:C:107:LYS:HE2	1:C:111:ARG:NH2	2.32	0.43
1:C:33[B]:ILE:HD11	1:C:280:LEU:CD1	2.49	0.43
1:D:27:GLY:HA2	1:D:242:TYR:CE1	2.54	0.43
1:C:65:LEU:HD11	1:C:83:VAL:HG23	2.01	0.43
1:A:185:LYS:NZ	1:A:227:CYS:HB2	2.34	0.43
1:C:155:LEU:HD23	1:C:155:LEU:C	2.39	0.43
1:A:159:PRO:HG3	1:A:165:ASP:HA	2.01	0.42
1:D:154[B]:MSE:HE2	1:D:208:TYR:CD2	2.54	0.42
1:B:234:ILE:HG13	1:B:234:ILE:O	2.19	0.42
1:D:236:THR:N	3:D:317:MLT:C3	2.58	0.42
1:A:131:TRP:CH2	1:D:271:GLY:HA2	2.54	0.42
1:A:134:ASN:HD22	1:A:137:GLU:H	1.63	0.42
1:C:304:TYR:CE2	1:C:308:LEU:CD1	2.91	0.42
1:C:76:ASP:HB2	1:C:77:PRO:HD3	2.01	0.42
1:D:24:SER:CA	4:D:942:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:64:PRO:HD2	1:D:97:ILE:O	2.18	0.42
1:C:44:LEU:HB2	1:C:45:PRO:HD3	2.01	0.42
1:C:261:LEU:HD23	1:D:199:LEU:HD11	2.01	0.42
1:D:47:LEU:O	1:D:51:ILE:HG13	2.18	0.42
1:C:176:ARG:HG2	4:C:498:HOH:O	2.15	0.42
1:C:277:LYS:HE3	4:C:337:HOH:O	2.19	0.42
1:C:236:THR:OG1	3:C:317:MLT:O1	2.30	0.42
1:C:261:LEU:N	1:C:262:PRO:CD	2.83	0.42
1:C:251:GLU:HB2	4:C:382:HOH:O	2.19	0.42
1:B:97:ILE:O	1:B:97:ILE:HG23	2.19	0.41
1:D:33:ILE:CD1	1:D:33:ILE:C	2.87	0.41
1:C:33[A]:ILE:CD1	1:C:35:PRO:CD	2.96	0.41
1:A:220:VAL:HG23	1:A:221:ALA:N	2.35	0.41
1:B:33:ILE:C	1:B:33:ILE:CD1	2.89	0.41
1:C:47:LEU:O	1:C:51:ILE:HG13	2.20	0.41
1:A:131:TRP:HE3	1:A:132:LYS:N	2.18	0.41
1:D:270:ARG:HB2	1:D:275:THR:HG21	2.02	0.41
1:C:289:ALA:HB1	1:C:290:PRO:CD	2.50	0.41
1:D:155:LEU:HD23	1:D:156:TYR:N	2.35	0.41
1:D:217:GLU:HA	1:D:220[A]:VAL:CG2	2.50	0.41
1:D:250:LEU:HD11	1:D:254:ARG:NH1	2.34	0.41
1:C:234:ILE:HA	3:C:317:MLT:O2	2.21	0.41
1:D:242:TYR:CE2	1:D:246:LEU:HD11	2.56	0.41
1:C:105:THR:O	1:C:109:VAL:HG23	2.21	0.41
1:D:272:LEU:HB2	1:D:273:PRO:HD3	2.02	0.41
1:B:29:ILE:HG12	1:B:61:ALA:HB3	2.03	0.41
1:D:97:ILE:HD11	1:D:154[B]:MSE:HB3	2.02	0.41
1:B:217:GLU:O	1:B:220:VAL:CG2	2.69	0.41
1:D:216:LEU:HB2	1:D:257:PHE:CG	2.55	0.41
1:D:236:THR:CA	3:D:317:MLT:H31	2.49	0.41
1:A:130:TYR:CE2	1:D:72:ALA:CB	3.04	0.41
1:A:33:ILE:HD11	1:A:35:PRO:HG3	2.02	0.41
1:D:155:LEU:HD21	1:D:166:MSE:CE	2.51	0.41
1:D:272:LEU:O	1:D:276:ILE:HG12	2.22	0.40
1:A:79:TRP:CH2	1:A:111[B]:ARG:HB3	2.56	0.40
1:B:272:LEU:O	1:B:276:ILE:HG12	2.21	0.40
1:D:261:LEU:N	1:D:262:PRO:CD	2.84	0.40
1:C:196:LYS:HB3	1:C:196:LYS:HE2	1.92	0.40
1:A:184:VAL:O	1:A:207:PHE:HA	2.21	0.40
1:B:132:LYS:HD2	1:B:164:ILE:CD1	2.51	0.40
1:B:217:GLU:CA	1:B:220:VAL:HG22	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:ALA:N	1:B:231:PRO:HD2	2.35	0.40
1:A:198:ARG:HG2	1:B:258:TYR:CZ	2.57	0.40
1:C:178:VAL:CG1	1:C:181:VAL:HG23	2.52	0.40
1:C:217:GLU:O	1:C:220:VAL:HG23	2.18	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	293/315 (93%)	285 (97%)	8 (3%)	0	100	100
1	B	292/315 (93%)	286 (98%)	6 (2%)	0	100	100
1	C	290/315 (92%)	282 (97%)	8 (3%)	0	100	100
1	D	295/315 (94%)	291 (99%)	4 (1%)	0	100	100
All	All	1170/1260 (93%)	1144 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	237/245 (97%)	234 (99%)	3 (1%)	69	58
1	B	239/245 (98%)	238 (100%)	1 (0%)	91	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	234/245 (96%)	233 (100%)	1 (0%)	91 89
1	D	240/245 (98%)	240 (100%)	0	100 100
All	All	950/980 (97%)	945 (100%)	5 (0%)	88 86

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ARG
1	A	131	TRP
1	A	134	ASN
1	B	39	ASP
1	C	131	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	134	ASN
1	A	141	HIS
1	A	212	ASN
1	A	232	ASN
1	A	238	ASN
1	A	260	GLN
1	B	60	HIS
1	B	209	ASN
1	B	212	ASN
1	B	232	ASN
1	B	238	ASN
1	B	260	GLN
1	B	306	GLN
1	C	60	HIS
1	C	212	ASN
1	C	232	ASN
1	C	238	ASN
1	C	260	GLN
1	D	60	HIS
1	D	212	ASN
1	D	232	ASN
1	D	238	ASN
1	D	260	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	CSO	B	211	1	3,6,7	0.65	0	0,6,8	0.00	-
1	CSO	A	211	1	3,6,7	0.67	0	0,6,8	0.00	-
1	CSO	D	211	1	3,6,7	0.65	0	0,6,8	0.00	-
1	CSO	C	211	1	3,6,7	0.67	0	0,6,8	0.00	-

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
1	CSO	B	211	1	-	1/1/5/7	-
1	CSO	A	211	1	-	1/1/5/7	-
1	CSO	D	211	1	-	1/1/5/7	-
1	CSO	C	211	1	-	1/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	211	CSO	N-CA-CB-SG
1	B	211	CSO	N-CA-CB-SG
1	A	211	CSO	N-CA-CB-SG

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Mol	Chain	Res	Type	Atoms
1	D	211	CSO	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	211	CSO	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	$\#\|Z\| > 2$
3	MLT	C	317	-	2,8,8	0.23	0	3,10,10	0.89	0
3	MLT	D	317	-	2,8,8	0.19	0	3,10,10	0.82	0
3	MLT	A	317	-	2,8,8	0.26	0	3,10,10	0.97	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
3	MLT	C	317	-	-	0/2/8/8	-
3	MLT	D	317	-	-	2/2/8/8	-
3	MLT	A	317	-	-	0/2/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	317	MLT	C1-C2-C3-C4
3	D	317	MLT	O3-C2-C3-C4

There are no ring outliers.

3 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	317	MLT	2	0
3	D	317	MLT	16	0
3	A	317	MLT	1	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, 95^{th} 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	285/315 (90%)	0.26	7 (2%) 57 56	15, 22, 28, 36	0
1	B	284/315 (90%)	0.13	4 (1%) 75 76	16, 23, 30, 38	1 (0%)
1	C	285/315 (90%)	0.34	12 (4%) 36 34	22, 29, 36, 43	0
1	D	284/315 (90%)	0.34	8 (2%) 53 52	24, 29, 35, 43	2 (0%)
All	All	1138/1260 (90%)	0.27	31 (2%) 54 53	15, 26, 34, 43	3 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	131	TRP	7.1
1	A	131	TRP	6.3
1	A	130	TYR	4.4
1	A	38	ALA	3.8
1	C	204	ARG	3.7
1	C	130	TYR	3.5
1	C	38	ALA	3.4
1	C	303	ARG	3.3
1	C	39	ASP	3.2
1	A	161	THR	3.1
1	A	23	ALA	3.1
1	C	23	ALA	2.9
1	D	250	LEU	2.9
1	C	37	ALA	2.8
1	B	251	GLU	2.7
1	C	24	SER	2.7
1	C	252	LYS	2.4
1	D	39[A]	ASP	2.4
1	C	269	ARG	2.4
1	D	204	ARG	2.4
1	D	284	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	311	GLU	2.3
1	D	73	TYR	2.2
1	B	39	ASP	2.2
1	C	268	LEU	2.1
1	B	41	GLY	2.1
1	A	204	ARG	2.1
1	D	130	TYR	2.1
1	D	53	ARG	2.1
1	B	269	ARG	2.0
1	A	39	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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. The B-factors column lists the minimum, median, 95^{th} 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
1	CSO	A	211	7/8	0.89	0.13	21,21,22,23	0
1	CSO	C	211	7/8	0.91	0.12	28,28,29,30	0
1	CSO	D	211	7/8	0.92	0.11	27,27,28,29	0
1	CSO	B	211	7/8	0.93	0.10	20,20,22,23	0

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. The B-factors column lists the minimum, median, 95^{th} 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
3	MLT	A	317	9/9	0.79	0.19	36,36,36,36	0
3	MLT	D	317	9/9	0.81	0.25	42,43,43,43	0
3	MLT	C	317	9/9	0.82	0.22	56,56,56,56	0
2	MG	B	316	1/1	0.97	0.06	23,23,23,23	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MG	C	316	1/1	0.98	0.13	28,28,28,28	0
2	MG	A	316	1/1	0.98	0.16	22,22,22,22	0
2	MG	D	316	1/1	0.98	0.05	35,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.