



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:35 PM UTC

PDB ID : 5AA2 / pdb\_00005aa2  
Title : Crystal structure of MltF from *Pseudomonas aeruginosa* in complex with NAM-pentapeptide.  
Authors : Dominguez-Gil, T.; Acebron, I.; Hermoso, J.A.  
Deposited on : 2015-07-23  
Resolution : 2.80 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

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

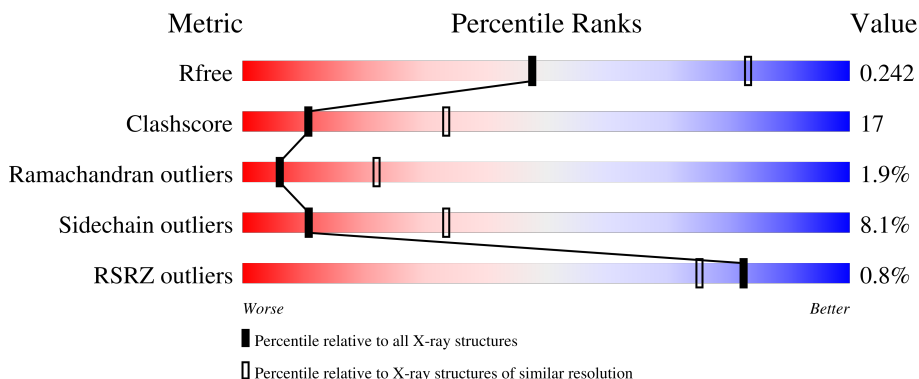
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	499	 59% 22% 17% 2% 2%
1	C	499	 62% 19% 16% 2% 2%
2	B	499	 56% 22% 17% 2% 2%
3	D	499	 52% 28% 17% 2% 2%
4	E	6	 17% 83% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
4	API	E	4	-	-	X	-
4	DAL	E	5	-	-	X	-
4	DAL	E	6	-	-	X	-

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 13519 atoms, of which 37 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 MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	419	3371	2126	599	637	9	0	1	0
1	C	418	3353	2114	597	633	9	0	0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP Q9HYN1
A	-20	ALA	-	expression tag	UNP Q9HYN1
A	-19	PRO	-	expression tag	UNP Q9HYN1
A	-18	SER	-	expression tag	UNP Q9HYN1
A	-17	ARG	-	expression tag	UNP Q9HYN1
A	-16	LEU	-	expression tag	UNP Q9HYN1
A	-15	CYS	-	expression tag	UNP Q9HYN1
A	-14	VAL	-	expression tag	UNP Q9HYN1
A	-13	TYR	-	expression tag	UNP Q9HYN1
A	-12	CYS	-	expression tag	UNP Q9HYN1
A	-11	ALA	-	expression tag	UNP Q9HYN1
A	-10	ASP	-	expression tag	UNP Q9HYN1
A	-9	VAL	-	expression tag	UNP Q9HYN1
A	-8	CYS	-	expression tag	UNP Q9HYN1
A	-7	PRO	-	expression tag	UNP Q9HYN1
A	-6	ASP	-	expression tag	UNP Q9HYN1
A	268	THR	ALA	conflict	UNP Q9HYN1
A	289	LYS	LEU	conflict	UNP Q9HYN1
A	446	SER	PRO	conflict	UNP Q9HYN1
C	-21	MET	-	expression tag	UNP Q9HYN1
C	-20	ALA	-	expression tag	UNP Q9HYN1
C	-19	PRO	-	expression tag	UNP Q9HYN1
C	-18	SER	-	expression tag	UNP Q9HYN1
C	-17	ARG	-	expression tag	UNP Q9HYN1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	LEU	-	expression tag	UNP Q9HXN1
C	-15	CYS	-	expression tag	UNP Q9HXN1
C	-14	VAL	-	expression tag	UNP Q9HXN1
C	-13	TYR	-	expression tag	UNP Q9HXN1
C	-12	CYS	-	expression tag	UNP Q9HXN1
C	-11	ALA	-	expression tag	UNP Q9HXN1
C	-10	ASP	-	expression tag	UNP Q9HXN1
C	-9	VAL	-	expression tag	UNP Q9HXN1
C	-8	CYS	-	expression tag	UNP Q9HXN1
C	-7	PRO	-	expression tag	UNP Q9HXN1
C	-6	ASP	-	expression tag	UNP Q9HXN1
C	268	THR	ALA	conflict	UNP Q9HXN1
C	289	LYS	LEU	conflict	UNP Q9HXN1
C	446	SER	PRO	conflict	UNP Q9HXN1

- Molecule 2 is a protein called MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	413	3309	2087	591	622	9	0	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	MET	-	expression tag	UNP Q9HXN1
B	-20	ALA	-	expression tag	UNP Q9HXN1
B	-19	PRO	-	expression tag	UNP Q9HXN1
B	-18	SER	-	expression tag	UNP Q9HXN1
B	-17	ARG	-	expression tag	UNP Q9HXN1
B	-16	LEU	-	expression tag	UNP Q9HXN1
B	-15	CYS	-	expression tag	UNP Q9HXN1
B	-14	VAL	-	expression tag	UNP Q9HXN1
B	-13	TYR	-	expression tag	UNP Q9HXN1
B	-12	CYS	-	expression tag	UNP Q9HXN1
B	-11	ALA	-	expression tag	UNP Q9HXN1
B	-10	ASP	-	expression tag	UNP Q9HXN1
B	-9	VAL	-	expression tag	UNP Q9HXN1
B	-8	CYS	-	expression tag	UNP Q9HXN1
B	-7	PRO	-	expression tag	UNP Q9HXN1
B	-6	ASP	-	expression tag	UNP Q9HXN1
B	161	PRO	GLU	conflict	UNP Q9HXN1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	268	THR	ALA	conflict	UNP Q9HYN1
B	289	LYS	LEU	conflict	UNP Q9HYN1

- Molecule 3 is a protein called MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	416	3334	2102	594	629	9	0	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-21	MET	-	expression tag	UNP Q9HYN1
D	-20	ALA	-	expression tag	UNP Q9HYN1
D	-19	PRO	-	expression tag	UNP Q9HYN1
D	-18	SER	-	expression tag	UNP Q9HYN1
D	-17	ARG	-	expression tag	UNP Q9HYN1
D	-16	LEU	-	expression tag	UNP Q9HYN1
D	-15	CYS	-	expression tag	UNP Q9HYN1
D	-14	VAL	-	expression tag	UNP Q9HYN1
D	-13	TYR	-	expression tag	UNP Q9HYN1
D	-12	CYS	-	expression tag	UNP Q9HYN1
D	-11	ALA	-	expression tag	UNP Q9HYN1
D	-10	ASP	-	expression tag	UNP Q9HYN1
D	-9	VAL	-	expression tag	UNP Q9HYN1
D	-8	CYS	-	expression tag	UNP Q9HYN1
D	-7	PRO	-	expression tag	UNP Q9HYN1
D	-6	ASP	-	expression tag	UNP Q9HYN1
D	102	ASP	GLU	conflict	UNP Q9HYN1
D	268	THR	ALA	conflict	UNP Q9HYN1
D	289	LYS	LEU	conflict	UNP Q9HYN1

- Molecule 4 is a protein called N-ACETYLGLUCOSAMINE-1,6-ANHYDRO-N-ACETYLMURAMIC ACID L-ALA-D-GLU-M-DAP-D-ALA-D-ALA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
4	E	6	79	24	37	6	12	0	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

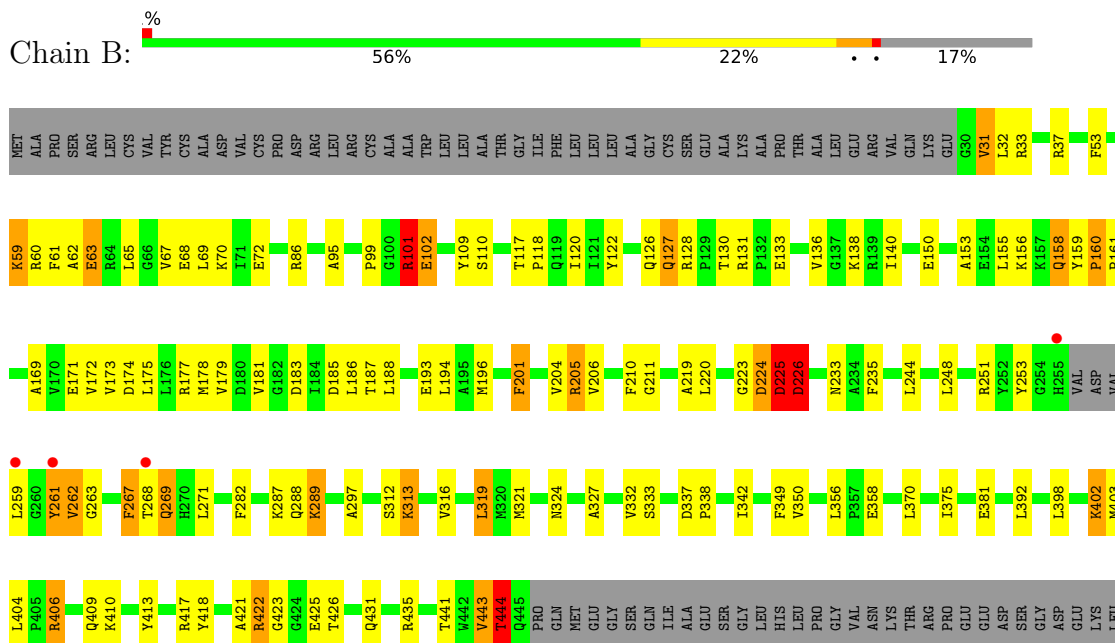
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	C	1	Total Cl 1 1	0	0

- Molecule 6 is water.

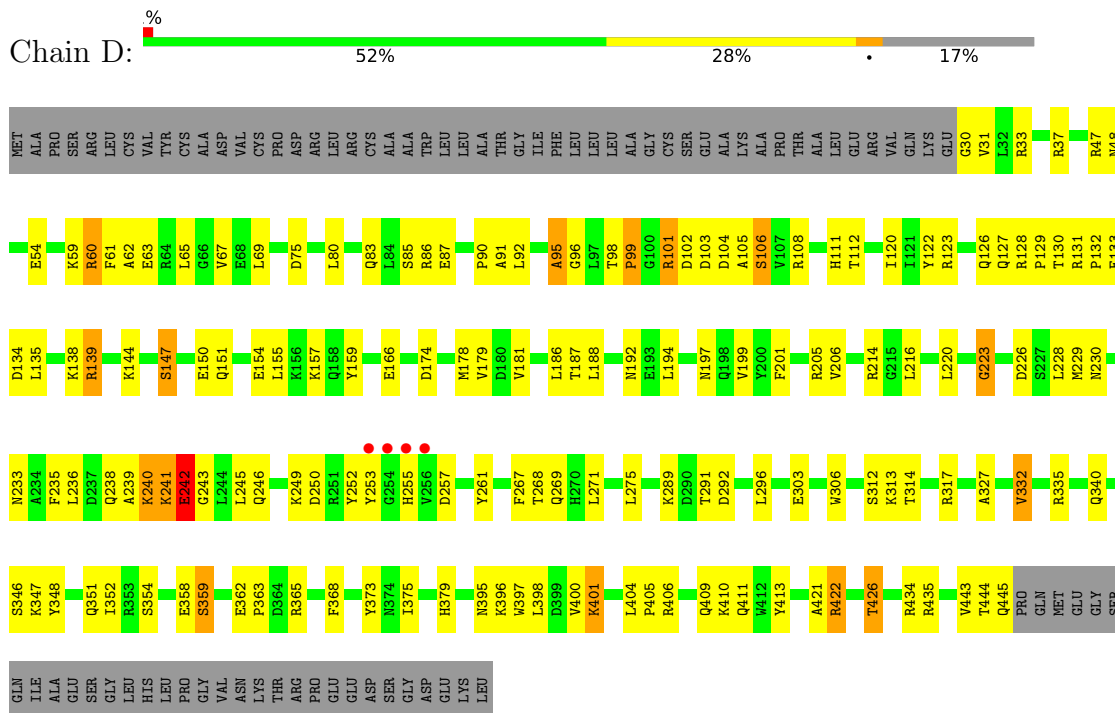
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	25	Total O 25 25	0	0
6	B	15	Total O 15 15	0	0
6	C	24	Total O 24 24	0	0
6	D	7	Total O 7 7	0	0



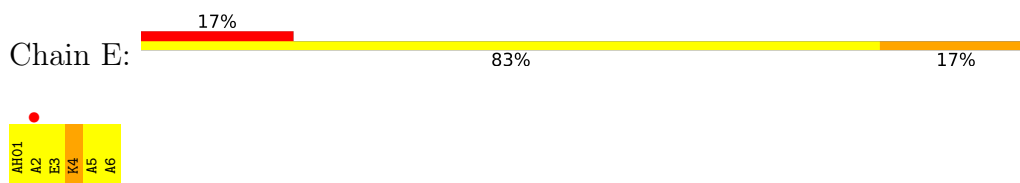
● Molecule 2: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F



● Molecule 3: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F



● Molecule 4: N-ACETYLGLUCOSAMINE-1,6-ANHYDRO-N-ACETYLMURAMIC ACID L-A LA-D-GLU-M-DAP-D-ALA-D-ALA



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.58Å 135.65Å 137.46Å 90.00° 92.06° 90.00°	Depositor
Resolution (Å)	48.26 – 2.80 48.26 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.26-2.80) 93.8 (48.26-2.80)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.167 , 0.235 0.180 , 0.242	Depositor DCC
$R_{free}$ test set	3153 reflections (5.34%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.0	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 41.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.004 for -h,l,k 0.016 for -h,-l,-k 0.034 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13519	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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: DGL, AH0, CL, DAL, API

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	0.60	0/3442	0.86	4/4652 (0.1%)
1	C	0.55	0/3423	0.84	5/4626 (0.1%)
2	B	0.53	0/3378	0.86	12/4564 (0.3%)
3	D	0.47	0/3404	0.81	2/4602 (0.0%)
4	E	0.89	0/4	0.94	0/4
All	All	0.54	0/13651	0.84	23/18448 (0.1%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	89	GLY	CA-C-N	7.43	127.47	119.89
1	A	89	GLY	C-N-CA	7.43	127.47	119.89
2	B	201	PHE	CA-C-N	6.28	127.69	119.84
2	B	201	PHE	C-N-CA	6.28	127.69	119.84
2	B	269	GLN	N-CA-C	-6.10	103.80	111.11
2	B	136	VAL	N-CA-C	5.97	116.71	110.62
2	B	117	THR	CA-C-N	-5.82	113.71	119.99
2	B	117	THR	C-N-CA	-5.82	113.71	119.99
1	C	201	PHE	CA-C-N	5.75	126.14	119.47
1	C	201	PHE	C-N-CA	5.75	126.14	119.47
2	B	160	PRO	N-CA-CB	5.60	108.51	103.08
2	B	225	ASP	CA-C-N	5.50	131.60	121.70
2	B	225	ASP	C-N-CA	5.50	131.60	121.70
2	B	101	ARG	CA-C-N	5.36	131.35	121.70
2	B	101	ARG	C-N-CA	5.36	131.35	121.70
3	D	201	PHE	CA-C-N	5.33	125.40	119.32
3	D	201	PHE	C-N-CA	5.33	125.40	119.32
2	B	267	PHE	N-CA-C	-5.24	103.57	110.43
1	C	393	ASN	CA-C-N	5.23	125.31	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	393	ASN	C-N-CA	5.23	125.31	119.87
1	A	159	TYR	CA-C-N	5.12	125.42	119.47
1	A	159	TYR	C-N-CA	5.12	125.42	119.47
1	C	31	VAL	N-CA-C	5.09	115.61	108.17

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	3371	0	3314	133	0
1	C	3353	0	3301	69	0
2	B	3309	0	3254	115	0
3	D	3334	0	3280	127	0
4	E	42	37	29	30	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	25	0	0	6	0
6	B	15	0	0	1	0
6	C	24	0	0	2	0
6	D	7	0	0	0	0
All	All	13482	37	13178	441	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 17.

All (441) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:ARG:HA	2:B:102:GLU:HB2	1.21	1.14
2:B:60:ARG:HD2	2:B:244:LEU:HD21	1.35	1.04
3:D:220:LEU:HD22	3:D:229:MET:HE2	1.36	1.03
2:B:101:ARG:HA	2:B:102:GLU:CB	1.94	0.98
1:C:144:LYS:HA	1:C:166:GLU:HB2	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:225:ASP:HA	2:B:226:ASP:HB2	1.44	0.96
3:D:241:LYS:N	3:D:242:GLU:HB2	1.80	0.96
2:B:101:ARG:CA	2:B:102:GLU:HB2	1.99	0.91
1:A:29:GLU:HG2	1:A:30:GLY:H	1.36	0.91
2:B:101:ARG:HG3	2:B:101:ARG:HH11	1.38	0.88
2:B:268:THR:HA	2:B:271:LEU:HB3	1.52	0.87
3:D:104:ASP:O	3:D:106:SER:N	2.05	0.87
2:B:225:ASP:HA	2:B:226:ASP:CB	2.04	0.87
3:D:268:THR:HA	3:D:271:LEU:HB2	1.54	0.87
1:A:37:ARG:HH22	4:E:4:API:C	1.88	0.86
1:A:172:VAL:HG21	4:E:4:API:H41	1.57	0.85
1:A:98:THR:O	4:E:2:ALA:HB3	1.76	0.84
1:A:249:LYS:O	1:A:253[B]:TYR:HB2	1.76	0.83
3:D:241:LYS:HB2	3:D:242:GLU:CG	2.08	0.83
1:A:196:MET:HB2	1:A:253[A]:TYR:CE1	2.14	0.82
3:D:197:ASN:OD1	3:D:422:ARG:NH2	2.13	0.81
3:D:101:ARG:HE	3:D:101:ARG:HA	1.46	0.81
1:C:289:LYS:HB2	1:C:289:LYS:NZ	1.96	0.80
3:D:242:GLU:HB3	3:D:243:GLY:HA2	1.61	0.80
1:A:102:GLU:HA	1:A:103:ASP:O	1.82	0.80
2:B:422:ARG:HG2	2:B:425:GLU:HG2	1.64	0.79
3:D:192:ASN:HB2	3:D:253:TYR:HE2	1.48	0.78
2:B:268:THR:HA	2:B:271:LEU:CB	2.12	0.78
1:A:29:GLU:CG	1:A:30:GLY:H	1.97	0.77
2:B:31:VAL:HA	2:B:67:VAL:CG2	2.14	0.77
1:A:172:VAL:HG21	4:E:4:API:C4	2.14	0.77
2:B:261:TYR:O	2:B:263:GLY:N	2.17	0.76
2:B:313:LYS:HE2	2:B:313:LYS:H	1.48	0.76
2:B:196:MET:HE3	2:B:253:TYR:CE1	2.20	0.75
1:A:226:ASP:O	1:A:230:ASN:ND2	2.18	0.75
2:B:289:LYS:HB2	2:B:289:LYS:NZ	2.01	0.75
3:D:242:GLU:CB	3:D:243:GLY:HA2	2.15	0.73
3:D:261:TYR:CE1	3:D:435:ARG:HG2	2.23	0.73
1:A:120:ILE:HD13	1:A:188:LEU:HD13	1.69	0.72
3:D:246:GLN:HE22	3:D:249:LYS:HE2	1.52	0.72
2:B:225:ASP:CA	2:B:226:ASP:HB2	2.19	0.72
3:D:101:ARG:HG3	3:D:102:ASP:O	1.88	0.72
3:D:154:GLU:O	3:D:157:LYS:HG2	1.88	0.71
2:B:60:ARG:HA	2:B:63:GLU:HG2	1.72	0.71
2:B:102:GLU:HA	2:B:102:GLU:OE1	1.89	0.71
3:D:108:ARG:NH2	3:D:223:GLY:HA2	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ASN:HD21	4:E:5:DAL:HB3	1.56	0.70
1:A:444:THR:HG22	1:A:445:GLN:H	1.55	0.70
2:B:101:ARG:HH11	2:B:101:ARG:CG	2.04	0.70
1:A:98:THR:HB	4:E:2:ALA:CB	2.22	0.70
3:D:192:ASN:HB2	3:D:253:TYR:CE2	2.27	0.69
1:A:96:GLY:HA3	4:E:5:DAL:C	2.22	0.69
2:B:224:ASP:O	2:B:226:ASP:HB2	1.92	0.69
3:D:397:TRP:O	3:D:401:LYS:HB3	1.92	0.69
3:D:91:ALA:HB1	3:D:228:LEU:CD2	2.23	0.69
3:D:271:LEU:HD23	3:D:275:LEU:HD22	1.73	0.69
3:D:91:ALA:HB1	3:D:228:LEU:HD21	1.75	0.68
1:A:84:LEU:O	1:A:221:PRO:HG3	1.94	0.68
1:C:220:LEU:HD22	1:C:229:MET:HE2	1.76	0.68
1:A:172:VAL:CG2	4:E:4:API:H41	2.22	0.68
2:B:443:VAL:O	2:B:443:VAL:HG12	1.94	0.67
3:D:102:ASP:C	3:D:104:ASP:H	2.02	0.67
2:B:158:GLN:HG2	2:B:159:TYR:CD1	2.29	0.67
1:A:256:VAL:HG11	1:A:313:LYS:NZ	2.09	0.67
3:D:239:ALA:C	3:D:240:LYS:HZ1	2.02	0.67
3:D:241:LYS:H	3:D:242:GLU:HB2	1.59	0.67
1:A:54:GLU:HG2	4:E:6:DAL:HB2	1.76	0.66
3:D:226:ASP:O	3:D:230:ASN:HB2	1.95	0.66
2:B:251:ARG:HH11	2:B:251:ARG:HG2	1.61	0.66
1:C:122:TYR:CZ	1:C:128:ARG:HG3	2.31	0.66
3:D:327:ALA:HB1	3:D:332:VAL:HG22	1.77	0.66
1:A:311:THR:CG2	1:A:317:ARG:HE	2.09	0.65
2:B:61:PHE:HB2	2:B:235:PHE:CE2	2.31	0.65
2:B:204:VAL:O	2:B:205:ARG:HD3	1.96	0.65
2:B:177:ARG:NH1	2:B:409:GLN:HG2	2.11	0.65
1:C:427:VAL:O	1:C:431:GLN:HG2	1.98	0.64
3:D:104:ASP:C	3:D:106:SER:H	2.06	0.64
1:A:196:MET:HE1	1:A:252:TYR:HB3	1.79	0.64
1:C:80:LEU:HD23	1:C:80:LEU:C	2.23	0.64
1:A:122:TYR:CE1	1:A:128:ARG:HG3	2.33	0.63
3:D:241:LYS:HB2	3:D:242:GLU:CB	2.27	0.63
1:C:101:ARG:HG2	1:C:101:ARG:HH11	1.63	0.62
1:A:37:ARG:HD2	1:A:171:GLU:OE2	1.98	0.62
1:A:30:GLY:HA2	1:A:67:VAL:HG12	1.81	0.62
1:A:289:LYS:HE3	1:A:346:SER:C	2.25	0.62
3:D:312:SER:OG	3:D:314:THR:OG1	2.17	0.62
1:A:147:SER:HB3	4:E:3:DGL:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:GLU:HG2	6:A:2004:HOH:O	1.99	0.61
1:A:311:THR:HG23	1:A:317:ARG:HG3	1.82	0.61
3:D:229:MET:SD	3:D:233:ASN:ND2	2.73	0.61
3:D:240:LYS:HE3	3:D:245:LEU:HD11	1.82	0.61
1:A:98:THR:HB	4:E:2:ALA:HB1	1.82	0.61
2:B:131:ARG:HB2	2:B:133:GLU:HG2	1.82	0.61
1:A:122:TYR:CZ	1:A:128:ARG:HG3	2.35	0.61
1:C:261:TYR:CE1	1:C:435:ARG:HD3	2.36	0.61
3:D:60:ARG:NH1	3:D:63:GLU:OE1	2.33	0.61
1:C:92:LEU:HD12	1:C:92:LEU:C	2.25	0.61
1:A:196:MET:HB2	1:A:253[A]:TYR:CD1	2.35	0.60
2:B:185:ASP:O	2:B:186:LEU:HD23	2.00	0.60
2:B:31:VAL:HA	2:B:67:VAL:HG22	1.81	0.60
3:D:133:GLU:HG3	3:D:159:TYR:CZ	2.35	0.60
1:A:54:GLU:HG2	4:E:6:DAL:CB	2.31	0.60
2:B:313:LYS:H	2:B:313:LYS:CE	2.12	0.60
1:C:289:LYS:HB2	1:C:289:LYS:HZ2	1.66	0.60
2:B:60:ARG:HA	2:B:63:GLU:CG	2.32	0.60
2:B:289:LYS:HB2	2:B:289:LYS:HZ2	1.65	0.60
2:B:319:LEU:HD12	2:B:319:LEU:O	2.02	0.59
2:B:60:ARG:CD	2:B:244:LEU:HD21	2.23	0.59
1:C:79:ASP:O	1:C:83:GLN:HG2	2.01	0.59
1:C:378:ALA:HB1	1:C:418:TYR:CE2	2.37	0.59
1:A:98:THR:OG1	6:A:2007:HOH:O	2.16	0.59
3:D:132:PRO:O	3:D:135:LEU:HG	2.03	0.59
3:D:220:LEU:CD2	3:D:229:MET:HE2	2.22	0.59
1:A:146:SER:HA	4:E:3:DGL:OXT	2.03	0.59
1:A:254:GLY:O	1:A:256:VAL:HG22	2.01	0.59
2:B:128:ARG:HH12	2:B:130:THR:HG22	1.68	0.59
1:A:117:THR:O	1:A:191:SER:HB3	2.02	0.58
1:C:28:LYS:HZ3	1:C:28:LYS:N	2.02	0.58
1:A:102:GLU:N	1:A:103:ASP:HB2	2.18	0.58
2:B:59:LYS:HA	2:B:69:LEU:HD22	1.85	0.58
1:C:174:ASP:O	1:C:178:MET:HG3	2.03	0.58
1:C:443:VAL:O	1:C:443:VAL:HG23	2.03	0.58
3:D:242:GLU:HB3	3:D:243:GLY:CA	2.32	0.58
1:A:256:VAL:HG11	1:A:313:LYS:HZ3	1.68	0.58
1:A:192:ASN:ND2	4:E:5:DAL:HB3	2.19	0.58
1:C:261:TYR:CD1	1:C:435:ARG:HD3	2.38	0.58
3:D:296:LEU:HD13	3:D:346:SER:OG	2.03	0.58
1:A:325:ARG:HH11	1:A:325:ARG:CG	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:122:TYR:CE1	3:D:205:ARG:HB2	2.39	0.57
3:D:150:GLU:O	3:D:154:GLU:HG2	2.04	0.57
3:D:240:LYS:HB3	3:D:245:LEU:HG	1.86	0.57
2:B:99:PRO:HB3	2:B:109:TYR:CG	2.39	0.57
1:A:137:GLY:C	1:A:138:LYS:HD2	2.30	0.57
1:A:29:GLU:CG	1:A:30:GLY:N	2.67	0.57
3:D:241:LYS:HB2	3:D:242:GLU:HG3	1.85	0.57
3:D:267:PHE:O	3:D:268:THR:OG1	2.21	0.57
3:D:96:GLY:HA2	3:D:216:LEU:HD13	1.87	0.57
1:A:220:LEU:HD22	1:A:229:MET:HE2	1.86	0.56
3:D:268:THR:HA	3:D:271:LEU:CB	2.30	0.56
2:B:313:LYS:H	2:B:313:LYS:CD	2.17	0.56
2:B:402:LYS:HD2	2:B:402:LYS:N	2.20	0.56
1:C:378:ALA:HB1	1:C:418:TYR:CD2	2.39	0.56
1:C:393:ASN:ND2	1:C:396:LYS:HG2	2.19	0.56
3:D:104:ASP:O	3:D:106:SER:OG	2.22	0.56
3:D:238:GLN:O	3:D:242:GLU:HG3	2.05	0.56
3:D:220:LEU:HD22	3:D:229:MET:HB2	1.87	0.56
2:B:233:ASN:OD1	6:B:2008:HOH:O	2.18	0.56
1:A:54:GLU:CG	4:E:6:DAL:HB2	2.36	0.56
1:C:122:TYR:CE1	1:C:128:ARG:HG3	2.41	0.56
1:C:289:LYS:HB2	1:C:289:LYS:HZ3	1.70	0.56
1:A:121:ILE:CG2	1:A:204:VAL:HG13	2.36	0.55
3:D:246:GLN:NE2	3:D:249:LYS:HE2	2.20	0.55
2:B:183:ASP:O	3:D:411:GLN:HG2	2.06	0.55
2:B:194:LEU:CD2	2:B:206:VAL:HG22	2.37	0.55
4:E:1:AH0:HB3	4:E:2:ALA:HA	1.87	0.55
1:A:251:ARG:O	1:A:251:ARG:HG3	2.07	0.55
1:A:253[A]:TYR:OH	4:E:6:DAL:OXT	2.10	0.55
1:A:102:GLU:H	1:A:103:ASP:HB2	1.72	0.55
1:A:169:ALA:CB	1:C:139:ARG:HD2	2.37	0.55
2:B:251:ARG:HG2	2:B:251:ARG:NH1	2.21	0.55
1:A:37:ARG:NH2	4:E:4:API:C	2.64	0.54
1:C:134:ASP:O	1:C:138:LYS:HE2	2.06	0.54
2:B:118:PRO:HB2	2:B:210:PHE:O	2.08	0.54
3:D:289:LYS:HE3	3:D:347:LYS:N	2.23	0.54
3:D:240:LYS:CE	3:D:245:LEU:HD11	2.38	0.54
1:C:223:GLY:HA3	6:C:2009:HOH:O	2.07	0.54
2:B:128:ARG:NH1	2:B:130:THR:HG22	2.23	0.54
1:C:443:VAL:O	1:C:444:THR:HG23	2.07	0.54
1:A:291:THR:CG2	1:A:353:ARG:HH22	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:VAL:HG21	1:C:175:LEU:HD21	1.90	0.54
3:D:108:ARG:HH21	3:D:223:GLY:HA2	1.73	0.54
1:A:148:HIS:CE1	4:E:4:API:H52	2.43	0.54
1:C:271:LEU:CD1	1:C:275:LEU:HD23	2.38	0.54
3:D:252:TYR:C	3:D:253:TYR:HD1	2.16	0.54
2:B:267:PHE:O	2:B:268:THR:OG1	2.21	0.53
3:D:75:ASP:O	3:D:410:LYS:NZ	2.24	0.53
3:D:240:LYS:HE3	3:D:245:LEU:CD1	2.38	0.53
1:A:138:LYS:HD2	1:A:138:LYS:N	2.23	0.53
1:C:238:GLN:O	1:C:242:GLU:HB2	2.08	0.53
1:C:417:ARG:HD2	1:C:418:TYR:CE2	2.44	0.53
3:D:134:ASP:O	3:D:138:LYS:NZ	2.32	0.53
3:D:249:LYS:O	3:D:253:TYR:HB2	2.08	0.53
1:A:289:LYS:HE3	1:A:347:LYS:N	2.22	0.53
1:C:264:ALA:O	1:C:268:THR:HG23	2.08	0.53
3:D:102:ASP:O	3:D:104:ASP:N	2.38	0.53
1:A:172:VAL:CG2	4:E:4:API:C4	2.84	0.53
2:B:262:VAL:HG23	2:B:263:GLY:N	2.24	0.53
1:C:122:TYR:CE1	1:C:205:ARG:HB2	2.44	0.53
1:A:42:THR:O	1:A:54:GLU:HB2	2.09	0.53
2:B:381:GLU:OE1	2:B:381:GLU:HA	2.10	0.52
1:A:300:GLY:HA3	1:A:320:MET:CE	2.40	0.52
2:B:175:LEU:HD13	2:B:187:THR:OG1	2.10	0.52
2:B:289:LYS:HB2	2:B:289:LYS:HZ3	1.74	0.52
3:D:144:LYS:HE2	3:D:166:GLU:HB2	1.91	0.52
3:D:239:ALA:CA	3:D:240:LYS:HZ1	2.22	0.52
1:A:311:THR:HG23	1:A:317:ARG:HE	1.73	0.52
2:B:60:ARG:HD2	2:B:244:LEU:CD2	2.25	0.52
2:B:337:ASP:OD1	2:B:338:PRO:HD2	2.09	0.52
1:C:316:VAL:HA	1:C:322:LEU:O	2.10	0.52
3:D:131:ARG:HD2	3:D:133:GLU:OE1	2.10	0.52
1:A:144:LYS:HD2	1:A:145:GLY:N	2.25	0.52
3:D:359:SER:HB2	3:D:395:ASN:ND2	2.25	0.52
3:D:255:HIS:ND1	3:D:313:LYS:HE2	2.25	0.52
3:D:138:LYS:HD2	3:D:186:LEU:HD11	1.92	0.51
1:A:54:GLU:OE1	1:A:94:ALA:HB1	2.11	0.51
1:A:120:ILE:CD1	1:A:188:LEU:HD13	2.38	0.51
2:B:282:PHE:CZ	2:B:297:ALA:HA	2.45	0.51
1:A:135:LEU:CD2	1:A:186:LEU:HD13	2.39	0.51
1:A:291:THR:CG2	1:A:353:ARG:NH2	2.73	0.51
2:B:31:VAL:HG22	2:B:68:GLU:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:ARG:HD2	2:B:171:GLU:OE2	2.10	0.51
3:D:317:ARG:HB3	3:D:335:ARG:HH21	1.76	0.51
2:B:375:ILE:HB	2:B:426:THR:OG1	2.11	0.51
3:D:102:ASP:C	3:D:104:ASP:N	2.68	0.51
3:D:220:LEU:HD13	3:D:229:MET:CE	2.40	0.51
2:B:158:GLN:HG2	2:B:159:TYR:HD1	1.74	0.51
3:D:362:GLU:HB3	3:D:363:PRO:HA	1.93	0.51
1:A:101:ARG:O	1:A:102:GLU:HG3	2.11	0.51
1:A:200:TYR:OH	1:A:257:ASP:HB2	2.11	0.51
2:B:443:VAL:O	2:B:444:THR:HG23	2.11	0.51
1:C:271:LEU:HD12	1:C:275:LEU:HD23	1.92	0.51
3:D:275:LEU:HB2	3:D:306:TRP:CZ3	2.46	0.50
1:A:174:ASP:O	1:A:178:MET:HG3	2.10	0.50
1:C:133:GLU:HG3	1:C:159:TYR:CD2	2.46	0.50
1:A:378:ALA:HB1	1:A:418:TYR:CE2	2.47	0.50
1:A:347:LYS:HE3	2:B:358:GLU:OE2	2.10	0.50
2:B:122:TYR:CE1	2:B:205:ARG:HB3	2.46	0.50
2:B:126:GLN:O	2:B:127:GLN:HB2	2.12	0.50
3:D:379:HIS:CE1	3:D:421:ALA:HB2	2.46	0.50
1:A:325:ARG:NH1	1:A:325:ARG:HG3	2.27	0.50
2:B:169:ALA:CB	3:D:139:ARG:HD3	2.42	0.50
2:B:223:GLY:O	2:B:224:ASP:HB2	2.11	0.50
3:D:92:LEU:C	3:D:92:LEU:HD12	2.37	0.50
2:B:219:ALA:C	2:B:220:LEU:HD12	2.37	0.49
1:A:98:THR:HB	4:E:2:ALA:HB3	1.94	0.49
1:A:220:LEU:HD13	1:A:229:MET:CE	2.41	0.49
2:B:101:ARG:HA	2:B:102:GLU:CG	2.42	0.49
1:A:325:ARG:HH11	1:A:325:ARG:CB	2.25	0.49
1:C:194:LEU:O	1:C:198:GLN:HB2	2.12	0.49
1:C:275:LEU:HD12	1:C:275:LEU:O	2.12	0.49
3:D:375:ILE:HB	3:D:426:THR:OG1	2.11	0.49
3:D:54:GLU:HG3	3:D:95:ALA:HA	1.95	0.49
3:D:268:THR:HA	3:D:271:LEU:HD12	1.93	0.49
3:D:347:LYS:O	3:D:351:GLN:HB2	2.12	0.49
1:A:444:THR:HG22	1:A:445:GLN:N	2.25	0.49
1:C:108:ARG:HD2	6:C:2010:HOH:O	2.11	0.49
1:A:143:LEU:HB2	4:E:4:API:O3	2.13	0.49
2:B:244:LEU:HD12	2:B:244:LEU:O	2.13	0.49
1:A:170:VAL:HG22	1:A:174:ASP:CB	2.43	0.49
2:B:33:ARG:HD2	2:B:72:GLU:OE2	2.13	0.49
2:B:403:MET:O	2:B:406:ARG:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:404:LEU:HB2	3:D:405:PRO:HD3	1.95	0.49
2:B:120:ILE:HD13	2:B:188:LEU:HD13	1.95	0.48
1:A:177:ARG:HD3	6:A:2011:HOH:O	2.14	0.48
2:B:268:THR:OG1	2:B:269:GLN:N	2.46	0.48
1:C:37:ARG:NH1	1:C:171:GLU:OE2	2.45	0.48
3:D:147:SER:O	3:D:151:GLN:HG3	2.14	0.48
2:B:268:THR:HA	2:B:271:LEU:HB2	1.95	0.48
1:A:143:LEU:HD13	4:E:4:API:O3	2.13	0.48
3:D:83:GLN:O	3:D:90:PRO:HD2	2.14	0.48
3:D:220:LEU:HD13	3:D:229:MET:HE1	1.95	0.48
2:B:289:LYS:NZ	2:B:289:LYS:CB	2.71	0.48
1:C:289:LYS:NZ	1:C:289:LYS:CB	2.73	0.48
1:A:325:ARG:CG	1:A:325:ARG:NH1	2.77	0.48
1:C:104:ASP:OD2	1:C:106:SER:HB2	2.13	0.48
1:C:138:LYS:HG3	1:C:186:LEU:HD11	1.96	0.48
3:D:133:GLU:HG3	3:D:159:TYR:CE2	2.49	0.48
3:D:410:LYS:HA	3:D:413:TYR:CE2	2.49	0.48
2:B:133:GLU:HB3	2:B:159:TYR:HE2	1.77	0.47
3:D:120:ILE:HD13	3:D:188:LEU:HD13	1.95	0.47
2:B:53:PHE:CE2	2:B:248:LEU:HB3	2.50	0.47
2:B:404:LEU:O	2:B:423:GLY:HA3	2.14	0.47
1:C:397:TRP:CZ2	1:C:430:VAL:HG11	2.49	0.47
1:A:359:SER:HB2	1:A:395:ASN:OD1	2.14	0.47
3:D:240:LYS:HE3	3:D:240:LYS:HB3	1.68	0.47
1:A:156:LYS:HE3	1:A:162:LEU:O	2.15	0.47
4:E:5:DAL:O	4:E:6:DAL:HB3	2.15	0.47
3:D:354:SER:HA	3:D:365:ARG:HH21	1.80	0.47
1:A:289:LYS:HE3	1:A:347:LYS:HA	1.97	0.47
3:D:61:PHE:HD1	3:D:235:PHE:CG	2.33	0.47
3:D:268:THR:HG22	3:D:271:LEU:HD12	1.97	0.47
3:D:348:TYR:O	3:D:352:ILE:HG13	2.13	0.47
1:A:108:ARG:NH2	1:A:223:GLY:HA2	2.30	0.47
2:B:210:PHE:HA	2:B:211:GLY:HA2	1.54	0.47
2:B:31:VAL:CG1	2:B:32:LEU:N	2.76	0.46
2:B:312:SER:HA	2:B:313:LYS:HE2	1.97	0.46
2:B:327:ALA:HB1	2:B:332:VAL:CG1	2.45	0.46
1:A:271:LEU:O	1:A:276:PRO:HD3	2.14	0.46
1:C:443:VAL:O	1:C:443:VAL:CG2	2.62	0.46
3:D:241:LYS:CA	3:D:242:GLU:HB2	2.44	0.46
1:A:148:HIS:HD2	1:A:188:LEU:HG	1.79	0.46
1:A:192:ASN:ND2	4:E:6:DAL:OXT	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:VAL:HG13	1:C:340:GLN:HB3	1.98	0.46
1:A:172:VAL:HG21	4:E:4:API:H42	1.96	0.46
3:D:127:GLN:O	3:D:129:PRO:HD3	2.16	0.46
2:B:174:ASP:O	2:B:178:MET:HG3	2.16	0.46
3:D:174:ASP:O	3:D:178:MET:HG3	2.15	0.46
3:D:236:LEU:C	3:D:240:LYS:HZ3	2.23	0.46
3:D:239:ALA:HB3	3:D:240:LYS:HZ1	1.79	0.46
1:A:88:GLY:HA2	1:A:89:GLY:HA3	1.57	0.46
2:B:349:PHE:CE1	2:B:370:LEU:HD23	2.51	0.46
3:D:37:ARG:HG2	3:D:95:ALA:HB1	1.97	0.46
1:A:291:THR:HG21	1:A:353:ARG:NH2	2.30	0.46
2:B:194:LEU:HD21	2:B:206:VAL:HG22	1.97	0.46
1:C:277:ARG:HG2	1:C:277:ARG:HH11	1.81	0.45
1:A:180:ASP:OD1	1:A:203:ASN:HB2	2.17	0.45
1:A:379:HIS:O	1:A:382:ASP:HB2	2.15	0.45
1:C:241:LYS:HD2	1:C:241:LYS:HA	1.48	0.45
3:D:289:LYS:HB2	3:D:289:LYS:HZ3	1.82	0.45
2:B:443:VAL:O	2:B:443:VAL:CG1	2.63	0.45
2:B:338:PRO:O	2:B:342:ILE:HG13	2.16	0.45
2:B:413:TYR:CD1	2:B:413:TYR:C	2.94	0.45
1:C:77:LEU:HD23	1:C:77:LEU:HA	1.80	0.45
1:A:255:HIS:O	1:A:256:VAL:HG13	2.16	0.45
3:D:239:ALA:HB3	3:D:240:LYS:NZ	2.32	0.45
1:A:64:ARG:NH1	6:A:2004:HOH:O	2.50	0.45
1:C:36:THR:OG1	1:C:37:ARG:N	2.50	0.45
1:A:28:LYS:HB3	1:A:28:LYS:HE3	1.66	0.45
1:A:216:LEU:HD13	4:E:5:DAL:O	2.16	0.45
3:D:312:SER:C	3:D:314:THR:H	2.25	0.45
2:B:313:LYS:HE2	2:B:313:LYS:N	2.25	0.44
1:A:53:PHE:CD1	1:A:53:PHE:C	2.95	0.44
2:B:251:ARG:HG2	2:B:251:ARG:O	2.17	0.44
2:B:267:PHE:C	2:B:268:THR:HG23	2.42	0.44
3:D:59:LYS:O	3:D:63:GLU:HG2	2.17	0.44
1:C:185:ASP:O	1:C:186:LEU:HD23	2.17	0.44
2:B:59:LYS:O	2:B:62:ALA:HB3	2.18	0.44
3:D:122:TYR:CZ	3:D:128:ARG:HB2	2.53	0.44
2:B:402:LYS:HE3	2:B:402:LYS:HA	2.00	0.44
1:A:56:GLU:OE1	1:A:252:TYR:OH	2.35	0.44
2:B:159:TYR:CD1	2:B:159:TYR:N	2.85	0.44
2:B:316:VAL:HG23	2:B:321:MET:HE3	1.99	0.44
3:D:62:ALA:HB1	3:D:67:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:295:LEU:HD12	1:C:295:LEU:HA	1.79	0.44
3:D:268:THR:CA	3:D:271:LEU:HB2	2.38	0.44
1:A:325:ARG:HH11	1:A:325:ARG:HG3	1.82	0.44
1:A:238:GLN:HA	1:A:241:LYS:HG2	1.99	0.44
1:A:256:VAL:HG11	1:A:313:LYS:HZ1	1.83	0.44
1:C:254:GLY:HA3	1:C:313:LYS:NZ	2.33	0.44
1:C:311:THR:CG2	1:C:312:SER:N	2.81	0.44
1:C:401:LYS:NZ	1:C:401:LYS:HB3	2.33	0.44
1:A:293:TRP:CE2	1:A:294:ARG:HG3	2.53	0.43
1:A:300:GLY:HA3	1:A:320:MET:HE2	1.98	0.43
1:C:28:LYS:HA	1:C:29:GLU:HA	1.72	0.43
1:A:291:THR:HG22	1:A:353:ARG:HH22	1.82	0.43
2:B:101:ARG:CG	2:B:101:ARG:NH1	2.74	0.43
2:B:259:LEU:HD22	2:B:261:TYR:OH	2.18	0.43
1:C:277:ARG:HG2	1:C:277:ARG:NH1	2.34	0.43
3:D:86:ARG:HG2	3:D:87:GLU:OE1	2.18	0.43
3:D:271:LEU:CD2	3:D:275:LEU:HD22	2.44	0.43
2:B:392:LEU:HD23	2:B:392:LEU:HA	1.75	0.43
2:B:101:ARG:HG3	2:B:101:ARG:NH1	2.16	0.43
2:B:410:LYS:HA	2:B:413:TYR:CE2	2.52	0.43
1:C:301:TYR:CD1	1:C:305:LEU:HA	2.53	0.43
1:A:135:LEU:HD23	1:A:186:LEU:HD13	2.01	0.43
1:A:144:LYS:HD2	1:A:145:GLY:H	1.83	0.43
2:B:133:GLU:HA	2:B:159:TYR:CD2	2.53	0.43
3:D:31:VAL:HA	3:D:67:VAL:HG12	2.01	0.43
1:A:98:THR:C	4:E:2:ALA:HB3	2.43	0.43
2:B:172:VAL:HG11	2:B:193:GLU:HB3	2.01	0.43
2:B:262:VAL:CG2	2:B:263:GLY:N	2.81	0.43
3:D:317:ARG:HB3	3:D:335:ARG:NH2	2.34	0.43
1:A:35:ILE:HA	1:A:72:GLU:O	2.19	0.43
1:A:170:VAL:HG22	1:A:174:ASP:HB3	2.00	0.43
3:D:406:ARG:HA	3:D:409:GLN:HG3	2.01	0.43
1:A:148:HIS:CD2	1:A:188:LEU:HG	2.54	0.43
2:B:133:GLU:HB3	2:B:159:TYR:CE2	2.54	0.43
1:A:311:THR:HG21	1:A:317:ARG:HE	1.82	0.42
2:B:127:GLN:O	2:B:128:ARG:HB3	2.19	0.42
1:C:59:LYS:HA	1:C:69:LEU:HD22	1.99	0.42
3:D:80:LEU:C	3:D:80:LEU:HD23	2.44	0.42
3:D:111:HIS:HD1	3:D:233:ASN:CG	2.27	0.42
3:D:303:GLU:OE2	3:D:373:TYR:HE1	2.02	0.42
1:A:289:LYS:HE3	1:A:347:LYS:CA	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:288:GLN:O	2:B:288:GLN:HG2	2.20	0.42
1:A:41:ALA:O	4:E:6:DAL:HA	2.19	0.42
1:A:169:ALA:HB2	1:C:139:ARG:HD2	2.01	0.42
3:D:122:TYR:CE2	3:D:128:ARG:HB2	2.54	0.42
3:D:194:LEU:HD22	3:D:206:VAL:HG22	2.00	0.42
1:C:101:ARG:HG2	1:C:101:ARG:NH1	2.31	0.42
1:C:413:TYR:CD1	1:C:413:TYR:C	2.98	0.42
1:A:257:ASP:HB3	1:A:258:VAL:H	1.48	0.42
2:B:375:ILE:HD11	2:B:421:ALA:HB1	2.01	0.42
2:B:175:LEU:HD23	2:B:178:MET:CE	2.50	0.42
2:B:327:ALA:O	2:B:332:VAL:HB	2.19	0.42
1:C:314:THR:OG1	1:C:316:VAL:HG22	2.20	0.42
3:D:236:LEU:HA	3:D:240:LYS:HZ3	1.85	0.42
3:D:291:THR:CG2	3:D:292:ASP:N	2.83	0.42
3:D:396:LYS:HD3	3:D:396:LYS:HA	1.91	0.42
1:A:196:MET:CE	1:A:252:TYR:HB3	2.48	0.41
1:A:275:LEU:N	1:A:276:PRO:CD	2.83	0.41
1:A:275:LEU:HB3	1:A:276:PRO:HD3	2.02	0.41
2:B:150:GLU:HA	2:B:153:ALA:HB3	2.02	0.41
1:C:33:ARG:NE	1:C:72:GLU:OE2	2.43	0.41
3:D:47:ARG:HE	3:D:47:ARG:HB3	1.46	0.41
1:A:300:GLY:CA	1:A:320:MET:CE	2.98	0.41
2:B:267:PHE:O	2:B:268:THR:CB	2.66	0.41
3:D:123:ARG:O	3:D:126:GLN:HB2	2.20	0.41
3:D:267:PHE:O	3:D:269:GLN:N	2.51	0.41
1:C:121:ILE:HB	1:C:187:THR:HG22	2.01	0.41
1:A:135:LEU:HD23	1:A:186:LEU:CD1	2.51	0.41
1:A:282:PHE:HE1	1:A:320:MET:CE	2.34	0.41
1:C:275:LEU:N	1:C:276:PRO:CD	2.84	0.41
3:D:368:PHE:CZ	3:D:400:VAL:HG21	2.56	0.41
1:A:190:ASP:OD2	6:A:2007:HOH:O	2.22	0.41
1:C:364:ASP:HA	1:C:367:TRP:CD1	2.55	0.41
1:A:61:PHE:HB2	1:A:235:PHE:CE2	2.55	0.41
1:A:117:THR:O	1:A:191:SER:N	2.51	0.41
2:B:417:ARG:HD2	2:B:418:TYR:CE2	2.55	0.41
1:C:53:PHE:CE2	1:C:248:LEU:HB3	2.55	0.41
3:D:236:LEU:C	3:D:240:LYS:NZ	2.79	0.41
1:A:220:LEU:HD13	1:A:229:MET:HE2	2.02	0.41
1:A:410:LYS:HA	1:A:413:TYR:CE2	2.56	0.41
2:B:261:TYR:O	2:B:435:ARG:NH1	2.43	0.41
3:D:241:LYS:HB2	3:D:242:GLU:CA	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:241:LYS:HB2	3:D:242:GLU:HG2	1.97	0.41
3:D:291:THR:HG22	3:D:292:ASP:N	2.34	0.41
3:D:332:VAL:HB	3:D:340:GLN:HB3	2.02	0.41
1:A:36:THR:OG1	1:A:37:ARG:N	2.54	0.41
1:A:147:SER:CB	4:E:2:ALA:HB1	2.50	0.41
1:A:228:LEU:HB3	6:A:2008:HOH:O	2.20	0.41
1:A:244:LEU:O	1:A:244:LEU:HD22	2.20	0.41
2:B:140:ILE:HG12	2:B:186:LEU:HB2	2.03	0.41
2:B:160:PRO:N	2:B:161:PRO:CD	2.84	0.41
3:D:30:GLY:C	3:D:67:VAL:HG13	2.45	0.41
3:D:98:THR:HA	3:D:99:PRO:HD2	1.93	0.41
3:D:358:GLU:O	3:D:358:GLU:HG2	2.19	0.41
1:A:256:VAL:HB	1:A:257:ASP:H	1.45	0.40
1:A:291:THR:HG22	1:A:353:ARG:NH2	2.36	0.40
2:B:313:LYS:CD	2:B:313:LYS:N	2.83	0.40
1:C:42:THR:HG22	1:C:54:GLU:HG3	2.03	0.40
3:D:159:TYR:CD1	3:D:159:TYR:N	2.89	0.40
2:B:177:ARG:HA	2:B:201:PHE:CE1	2.56	0.40
1:C:287:LYS:C	1:C:289:LYS:H	2.30	0.40
1:A:303:GLU:OE1	1:A:321:MET:HB2	2.20	0.40
1:A:410:LYS:HA	1:A:413:TYR:CZ	2.57	0.40
3:D:179:VAL:HG21	3:D:187:THR:HG22	2.03	0.40
1:A:131:ARG:O	1:A:134:ASP:HB2	2.21	0.40
2:B:356:LEU:HD23	2:B:356:LEU:HA	1.89	0.40
1:C:266:THR:HG22	1:C:270:HIS:CE1	2.56	0.40
1:C:422:ARG:HG2	1:C:425:GLU:HG2	2.04	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	418/499 (84%)	390 (93%)	22 (5%)	6 (1%)	9	30
1	C	416/499 (83%)	385 (92%)	25 (6%)	6 (1%)	9	30
2	B	409/499 (82%)	374 (91%)	23 (6%)	12 (3%)	3	13
3	D	414/499 (83%)	379 (92%)	27 (6%)	8 (2%)	6	22
4	E	1/6 (17%)	1 (100%)	0	0	100	100
All	All	1658/2002 (83%)	1529 (92%)	97 (6%)	32 (2%)	6	22

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	VAL
2	B	102	GLU
2	B	262	VAL
3	D	105	ALA
1	A	29	GLU
1	A	104	ASP
1	A	257	ASP
2	B	95	ALA
2	B	101	ARG
2	B	127	GLN
2	B	158	GLN
2	B	226	ASP
2	B	261	TYR
2	B	444	THR
1	C	158	GLN
3	D	223	GLY
3	D	242	GLU
1	C	223	GLY
1	C	260	GLY
1	C	265	TYR
3	D	65	LEU
3	D	257	ASP
1	A	101	ARG
1	A	103	ASP
2	B	110	SER
2	B	224	ASP
1	C	258	VAL
3	D	95	ALA
1	C	198	GLN
2	B	443	VAL
3	D	99	PRO

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Mol	Chain	Res	Type
3	D	443	VAL

### 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	351/414 (85%)	325 (93%)	26 (7%)	13	37
1	C	349/414 (84%)	322 (92%)	27 (8%)	12	36
2	B	343/414 (83%)	313 (91%)	30 (9%)	9	30
3	D	347/414 (84%)	318 (92%)	29 (8%)	10	32
All	All	1390/1656 (84%)	1278 (92%)	112 (8%)	11	33

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	39	SER
1	A	76	ASN
1	A	87	GLU
1	A	101	ARG
1	A	102	GLU
1	A	120	ILE
1	A	130	THR
1	A	147	SER
1	A	170	VAL
1	A	194	LEU
1	A	199	VAL
1	A	244	LEU
1	A	256	VAL
1	A	257	ASP
1	A	287	LYS
1	A	311	THR
1	A	313	LYS
1	A	325	ARG
1	A	359	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	360	ILE
1	A	389	LYS
1	A	398	LEU
1	A	431	GLN
1	A	443	VAL
1	A	445	GLN
2	B	31	VAL
2	B	59	LYS
2	B	63	GLU
2	B	65	LEU
2	B	70	LYS
2	B	86	ARG
2	B	101	ARG
2	B	138	LYS
2	B	155	LEU
2	B	156	LYS
2	B	173	VAL
2	B	179	VAL
2	B	181	VAL
2	B	205	ARG
2	B	225	ASP
2	B	226	ASP
2	B	287	LYS
2	B	289	LYS
2	B	313	LYS
2	B	319	LEU
2	B	324	ASN
2	B	333	SER
2	B	350	VAL
2	B	398	LEU
2	B	402	LYS
2	B	406	ARG
2	B	422	ARG
2	B	431	GLN
2	B	441	THR
2	B	444	THR
1	C	28	LYS
1	C	39	SER
1	C	71	ILE
1	C	87	GLU
1	C	107	VAL
1	C	119	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	130	THR
1	C	150	GLU
1	C	158	GLN
1	C	196	MET
1	C	204	VAL
1	C	241	LYS
1	C	242	GLU
1	C	256	VAL
1	C	262	VAL
1	C	265	TYR
1	C	272	GLN
1	C	275	LEU
1	C	284	GLN
1	C	289	LYS
1	C	311	THR
1	C	317	ARG
1	C	341	SER
1	C	401	LYS
1	C	411	GLN
1	C	417	ARG
1	C	443	VAL
3	D	33	ARG
3	D	48	ASN
3	D	60	ARG
3	D	69	LEU
3	D	85	SER
3	D	101	ARG
3	D	103	ASP
3	D	106	SER
3	D	112	THR
3	D	130	THR
3	D	139	ARG
3	D	147	SER
3	D	155	LEU
3	D	181	VAL
3	D	199	VAL
3	D	214	ARG
3	D	240	LYS
3	D	241	LYS
3	D	242	GLU
3	D	250	ASP
3	D	332	VAL

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Mol	Chain	Res	Type
3	D	359	SER
3	D	398	LEU
3	D	401	LYS
3	D	422	ARG
3	D	426	THR
3	D	434	ARG
3	D	444	THR
3	D	445	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	GLN
2	B	127	GLN
2	B	158	GLN
2	B	269	GLN
1	C	340	GLN
3	D	238	GLN
3	D	281	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	$\# Z  > 2$
4	API	E	4	4	9,11,12	1.33	1 (11%)	5,13,15	1.41	1 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	API	E	4	4	-	8/11/12/14	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	4	API	O4-C7	-2.81	1.21	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	4	API	O4-C7-O3	-2.69	117.98	124.08

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	4	API	C4-C3-CA-C
4	E	4	API	C4-C3-CA-N
4	E	4	API	C4-C5-C6-C7
4	E	4	API	C4-C5-C6-N6
4	E	4	API	N6-C6-C7-O3
4	E	4	API	N6-C6-C7-O4
4	E	4	API	CA-C3-C4-C5
4	E	4	API	C3-C4-C5-C6

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	4	API	10	0

## 5.5 Carbohydrates i

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	419/499 (83%)	-0.77	2 (0%) 87 82	24, 45, 86, 156	1 (0%)
1	C	418/499 (83%)	-0.69	3 (0%) 84 77	29, 50, 92, 149	0
2	B	413/499 (82%)	-0.60	4 (0%) 79 72	30, 57, 93, 136	0
3	D	416/499 (83%)	-0.42	4 (0%) 79 72	38, 67, 110, 156	0
4	E	1/6 (16%)	3.50	1 (100%) 0 0	182, 182, 182, 182	0
All	All	1667/2002 (83%)	-0.62	14 (0%) 82 75	24, 56, 100, 182	1 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	256	VAL	4.1
1	A	256	VAL	3.6
1	C	259	LEU	3.6
4	E	2	ALA	3.5
3	D	256	VAL	2.9
2	B	268	THR	2.7
3	D	255	HIS	2.6
3	D	253	TYR	2.6
2	B	259	LEU	2.5
1	A	253[A]	TYR	2.5
2	B	255	HIS	2.5
3	D	254	GLY	2.4
1	C	258	VAL	2.3
2	B	261	TYR	2.2

### 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<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	B-factors( $\text{\AA}^2$ )	Q<0.9
4	DGL	E	3	9/10	0.88	0.23	118,144,167,173	0
4	API	E	4	12/13	0.90	0.21	133,186,235,282	0
4	DAL	E	6	6/6	0.91	0.21	109,124,146,163	0
4	DAL	E	5	5/6	0.93	0.22	142,147,175,177	0

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides 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<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	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CL	C	1446	1/1	0.92	0.23	100,100,100,100	0
5	CL	A	1446	1/1	0.95	0.10	61,61,61,61	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.