



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:45 pm BST

PDB ID : 3GMW
Title : Crystal Structure of Beta-Lactamase Inhibitory Protein-I (BLIP-I) in Complex with TEM-1 Beta-Lactamase
Authors : Lim, D.C.; Gretes, M.; Strynadka, N.C.J.
Deposited on : 2009-03-15
Resolution : 2.10 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 ⓘ](#)) 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

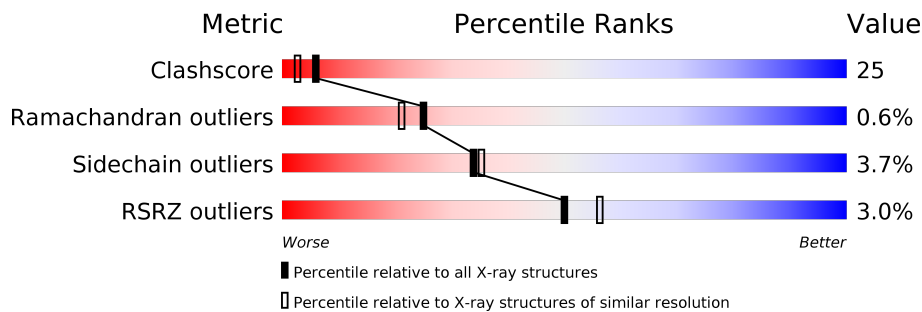
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 $\leq 5\%$. 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	261	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 70%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 23%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">3% 73% 23% •</p>
1	C	261	<div style="display: flex; align-items: center;"> <div style="width: 7%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 65%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 25%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">7% 72% 25% •</p>
2	B	156	<div style="display: flex; align-items: center;"> <div style="width: 82%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">82% 17% •</p>
2	D	156	<div style="display: flex; align-items: center;"> <div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">87% 12% •</p>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6861 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.

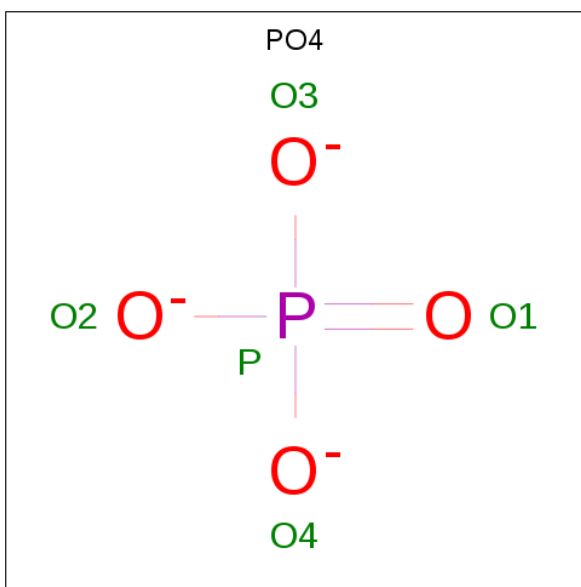
- Molecule 1 is a protein called B-lactamase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	261	Total 2023	C 1263	N 357	O 392	S 11	0	2	0
1	C	261	Total 2020	C 1261	N 359	O 389	S 11	0	1	0

- Molecule 2 is a protein called Beta-lactamase inhibitory protein BLIP-I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	154	Total 1205	C 770	N 190	O 239	S 6	0	0	0
2	D	156	Total 1221	C 779	N 192	O 244	S 6	0	1	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

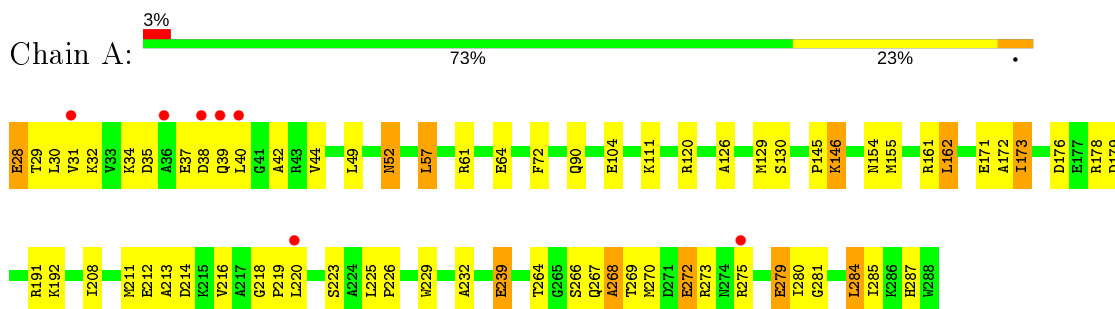
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	75	Total	O	0	0
			75	75		
4	B	106	Total	O	0	0
			106	106		
4	C	79	Total	O	0	0
			79	79		
4	D	112	Total	O	0	0
			112	112		

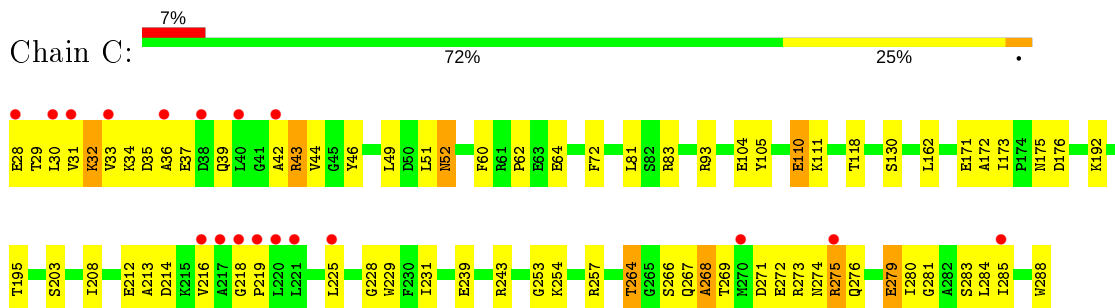
3 Residue-property plots [i](#)

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.

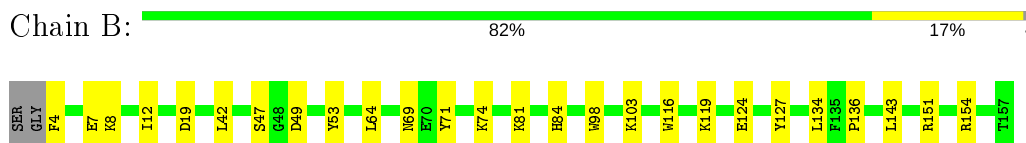
- Molecule 1: B-lactamase



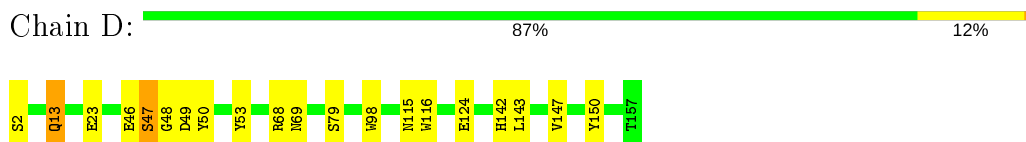
- Molecule 1: B-lactamase



- Molecule 2: Beta-lactamase inhibitory protein BLIP-I



- Molecule 2: Beta-lactamase inhibitory protein BLIP-I



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	45.42Å 48.76Å 106.14Å 103.24° 91.29° 90.18°	Depositor
Resolution (Å)	25.00 – 2.10 24.38 – 2.09	Depositor EDS
% Data completeness (in resolution range)	95.0 (25.00-2.10) 94.1 (24.38-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.99 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.192 , 0.234 0.185 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 29.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l 0.457 for -h,k,-k-l 0.029 for -h,-k,k+l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6861	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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: PO4

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	0.96	0/2061	0.94	3/2789 (0.1%)
1	C	0.95	1/2055 (0.0%)	0.94	2/2781 (0.1%)
2	B	1.23	1/1241 (0.1%)	1.02	4/1683 (0.2%)
2	D	1.21	1/1260 (0.1%)	1.01	2/1708 (0.1%)
All	All	1.06	3/6617 (0.0%)	0.97	11/8961 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	127	TYR	CD1-CE1	6.03	1.48	1.39
2	D	68	ARG	CG-CD	5.92	1.66	1.51
1	C	192	LYS	CE-NZ	5.67	1.63	1.49

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	49	ASP	CB-CG-OD2	7.18	124.76	118.30
2	D	49	ASP	CB-CG-OD2	7.06	124.65	118.30
1	A	120	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	C	49	LEU	CA-CB-CG	6.11	129.36	115.30
2	B	49	ASP	CB-CG-OD1	-5.93	112.96	118.30
2	B	19	ASP	CB-CG-OD1	5.72	123.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	49	ASP	CB-CG-OD1	-5.65	113.21	118.30
1	A	178	ARG	NE-CZ-NH1	-5.08	117.76	120.30
2	B	151	ARG	NE-CZ-NH1	-5.07	117.77	120.30
1	C	110	GLU	CA-CB-CG	5.02	124.45	113.40
1	A	162	LEU	CA-CB-CG	-5.01	103.77	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	28	GLU	Peptide

5.2 Too-close contacts [i](#)

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	2023	0	2036	190	0
1	C	2020	0	2037	193	0
2	B	1205	0	1111	31	0
2	D	1221	0	1125	12	0
3	B	10	0	0	0	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
4	A	75	0	0	3	0
4	B	106	0	0	10	0
4	C	79	0	0	3	0
4	D	112	0	0	4	0
All	All	6861	0	6309	318	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 25.

All (318) 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:A:31:VAL:HG22	1:C:31:VAL:CA	1.31	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:VAL:CG2	1:C:31:VAL:HA	1.38	1.49
1:A:30:LEU:HB3	1:C:30:LEU:CB	1.40	1.48
1:A:146:LYS:H	1:A:146:LYS:CD	1.23	1.47
1:A:31:VAL:CA	1:C:31:VAL:HG22	1.42	1.45
1:A:34:LYS:HE3	1:C:30:LEU:N	1.27	1.43
1:A:34:LYS:CE	1:C:30:LEU:H	1.35	1.39
1:A:31:VAL:HA	1:C:31:VAL:CG2	1.49	1.38
1:A:30:LEU:CB	1:C:30:LEU:HB3	1.56	1.32
1:A:34:LYS:HB3	1:C:28:GLU:CG	1.59	1.31
1:A:30:LEU:CB	1:C:30:LEU:CB	2.09	1.30
1:A:30:LEU:H	1:C:34:LYS:CE	1.48	1.27
1:A:30:LEU:N	1:C:34:LYS:HE2	1.49	1.25
1:A:30:LEU:HD22	1:C:30:LEU:HD13	1.27	1.16
1:C:269:THR:HG23	1:C:272:GLU:H	0.98	1.14
1:A:155:MET:HE2	1:A:192:LYS:HE3	1.26	1.14
1:A:31:VAL:CB	1:C:31:VAL:HG22	1.74	1.14
1:A:146:LYS:HD3	1:A:146:LYS:H	1.15	1.11
1:A:31:VAL:HG13	1:C:31:VAL:CG2	1.80	1.10
1:A:32:LYS:HE2	1:A:279:GLU:HB3	1.21	1.10
1:A:30:LEU:HD13	1:C:30:LEU:HD22	1.30	1.09
1:A:146:LYS:HD2	1:A:146:LYS:H	1.04	1.09
1:A:31:VAL:HG13	1:C:31:VAL:CG1	1.85	1.06
1:A:269:THR:OG1	1:A:272:GLU:HG2	1.55	1.06
1:A:30:LEU:CD2	1:C:30:LEU:HD13	1.84	1.06
1:A:146:LYS:CD	1:A:146:LYS:N	2.07	1.05
1:A:34:LYS:CD	1:C:28:GLU:HB2	1.87	1.05
1:A:30:LEU:HD22	1:C:30:LEU:CD1	1.85	1.05
1:A:30:LEU:HB3	1:C:30:LEU:HB2	1.07	1.04
1:A:34:LYS:HB3	1:C:28:GLU:HG3	1.10	1.04
1:A:31:VAL:CG1	1:C:31:VAL:HG13	1.91	1.00
1:A:30:LEU:HD13	1:C:30:LEU:CD2	1.91	1.00
1:A:30:LEU:HB2	1:C:30:LEU:HB3	1.37	1.00
1:A:31:VAL:CG1	1:C:31:VAL:HG22	1.90	0.99
1:A:146:LYS:HD2	1:A:146:LYS:N	1.70	0.99
1:A:34:LYS:HD3	1:C:28:GLU:HB2	1.41	0.98
1:C:36:ALA:HA	1:C:276:GLN:HE21	1.28	0.98
1:A:34:LYS:CG	1:C:28:GLU:HB2	1.93	0.97
1:A:31:VAL:HG22	1:C:31:VAL:CB	1.96	0.95
1:C:269:THR:HG23	1:C:272:GLU:N	1.79	0.95
1:A:155:MET:CE	1:A:192:LYS:HE3	1.96	0.95
1:A:28:GLU:N	1:A:287:HIS:HE1	1.63	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:LYS:HE3	1:C:279:GLU:HB3	1.49	0.94
1:A:281:GLY:HA2	1:A:284:LEU:CD1	1.99	0.93
1:A:31:VAL:HA	1:C:31:VAL:HG22	0.94	0.92
1:A:37:GLU:HG2	1:A:44:VAL:HG23	1.51	0.92
1:A:30:LEU:CD1	1:C:30:LEU:HD22	2.00	0.91
1:A:32:LYS:HE2	1:A:279:GLU:CB	2.00	0.91
1:A:34:LYS:CB	1:C:28:GLU:HG3	1.98	0.91
1:A:31:VAL:HA	1:C:31:VAL:HG23	1.50	0.91
1:A:155:MET:CE	1:A:192:LYS:CE	2.49	0.90
1:C:36:ALA:HA	1:C:276:GLN:NE2	1.84	0.90
1:C:269:THR:HG22	1:C:272:GLU:CG	2.02	0.90
1:A:220:LEU:O	1:A:223:SER:HB3	1.72	0.89
1:A:28:GLU:N	1:A:287:HIS:CE1	2.40	0.89
1:A:31:VAL:CG1	1:C:31:VAL:CG2	2.49	0.89
1:A:30:LEU:CB	1:C:30:LEU:HB2	1.88	0.88
1:A:30:LEU:CG	1:C:30:LEU:HD13	2.04	0.88
1:A:30:LEU:HD13	1:C:30:LEU:HD13	1.55	0.87
2:B:81:LYS:H	2:B:84:HIS:HD2	1.18	0.87
1:A:31:VAL:CG1	1:C:31:VAL:CG1	2.49	0.86
1:A:34:LYS:CB	1:C:28:GLU:CG	2.51	0.86
1:A:30:LEU:CD1	1:C:30:LEU:HD13	2.04	0.86
1:A:269:THR:H	1:A:272:GLU:CG	1.87	0.86
2:D:13:GLN:HG3	4:D:386:HOH:O	1.76	0.85
1:C:229:TRP:CZ3	1:C:285:ILE:HD12	2.11	0.85
1:C:36:ALA:CA	1:C:276:GLN:HE21	1.89	0.85
1:A:155:MET:HE2	1:A:192:LYS:CE	2.06	0.85
1:C:269:THR:CG2	1:C:272:GLU:H	1.87	0.84
1:A:218:GLY:N	1:A:219:PRO:HD3	1.94	0.83
1:A:30:LEU:HD13	1:C:30:LEU:CD1	2.08	0.82
1:A:30:LEU:HD13	1:C:30:LEU:CG	2.09	0.82
1:A:32:LYS:CE	1:A:279:GLU:HB3	2.08	0.82
1:C:243:ARG:HD3	1:C:273:ARG:NH1	1.95	0.82
1:A:42:ALA:HB1	1:A:264:THR:O	1.80	0.81
1:A:30:LEU:H	1:C:34:LYS:HE2	0.67	0.81
1:A:40:LEU:HD22	1:A:273:ARG:HG2	1.63	0.81
1:A:34:LYS:HD3	1:C:28:GLU:CB	2.11	0.80
1:C:28:GLU:N	1:C:31:VAL:CG2	2.44	0.80
1:A:29:THR:N	1:C:34:LYS:HE3	1.97	0.80
1:A:269:THR:H	1:A:272:GLU:HG3	1.44	0.80
1:C:267:GLN:O	1:C:268:ALA:O	1.99	0.79
1:A:31:VAL:HG13	1:C:31:VAL:CB	2.13	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LYS:HB3	1:C:28:GLU:HG2	1.63	0.78
2:B:81:LYS:H	2:B:84:HIS:CD2	2.01	0.78
1:A:145:PRO:HD2	1:A:146:LYS:HE3	1.66	0.78
1:C:280:ILE:O	1:C:283:SER:HB3	1.84	0.78
1:A:268:ALA:HB1	1:A:272:GLU:HG3	1.65	0.77
1:C:284:LEU:HB2	4:C:352:HOH:O	1.84	0.77
2:B:8:LYS:HE3	4:B:381:HOH:O	1.84	0.77
1:A:104[A]:GLU:OE2	2:B:154:ARG:NH1	2.18	0.76
2:B:4:PHE:CA	4:B:381:HOH:O	2.34	0.76
1:C:104:GLU:HG2	4:D:349:HOH:O	1.85	0.75
1:C:269:THR:HG22	1:C:272:GLU:CB	2.17	0.75
1:C:28:GLU:N	1:C:31:VAL:HG21	2.01	0.75
1:A:31:VAL:HG11	1:C:31:VAL:HG13	1.66	0.75
1:A:129:MET:HE1	2:B:42:LEU:HD23	1.69	0.75
1:C:111:LYS:HG2	1:C:111:LYS:O	1.86	0.75
1:C:43:ARG:HH21	1:C:264:THR:HG21	1.53	0.74
1:C:32:LYS:HE2	1:C:279:GLU:HG2	1.68	0.74
1:A:37:GLU:HG2	1:A:44:VAL:CG2	2.17	0.74
1:A:281:GLY:O	1:A:285:ILE:HG12	1.87	0.73
1:A:275:ARG:NH2	1:A:279:GLU:OE2	2.21	0.73
1:A:269:THR:N	1:A:272:GLU:HG3	2.03	0.73
1:A:31:VAL:CB	1:C:31:VAL:CG2	2.62	0.73
2:B:124:GLU:OE2	4:B:210:HOH:O	2.06	0.73
1:A:155:MET:HE1	1:A:192:LYS:CE	2.16	0.73
1:C:37:GLU:HG2	1:C:44:VAL:CG2	2.18	0.73
1:C:39:GLN:HG3	1:C:276:GLN:NE2	2.04	0.72
1:A:129:MET:CE	2:B:42:LEU:HD23	2.19	0.72
1:C:32:LYS:CE	1:C:279:GLU:HB3	2.19	0.71
1:C:213:ALA:O	1:C:214:ASP:C	2.29	0.70
1:C:46:TYR:OH	1:C:284:LEU:HD22	1.91	0.70
1:A:218:GLY:N	1:A:219:PRO:CD	2.54	0.70
1:C:36:ALA:CB	1:C:276:GLN:HE21	2.04	0.70
1:A:219:PRO:HG3	2:B:47:SER:HB2	1.72	0.69
1:C:46:TYR:OH	1:C:284:LEU:CD2	2.41	0.69
1:C:271:ASP:O	1:C:275:ARG:HB2	1.93	0.69
1:C:171:GLU:HA	1:C:239:GLU:HG3	1.73	0.69
1:C:219:PRO:HD3	2:D:47:SER:HB2	1.74	0.69
2:B:4:PHE:HA	4:B:381:HOH:O	1.91	0.68
1:C:269:THR:HG22	1:C:272:GLU:CD	2.12	0.68
1:A:173:ILE:N	1:A:173:ILE:HD13	2.07	0.68
1:A:34:LYS:HE2	1:C:30:LEU:HG	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:GLY:HA2	1:A:284:LEU:HD13	1.74	0.67
1:A:30:LEU:CG	1:C:30:LEU:HB3	2.25	0.67
1:A:34:LYS:HE2	1:C:30:LEU:CG	2.24	0.67
1:C:176:ASP:O	4:C:375:HOH:O	2.11	0.67
1:A:30:LEU:HB3	1:C:30:LEU:CG	2.22	0.67
1:C:28:GLU:N	1:C:31:VAL:HG23	2.10	0.67
1:A:28:GLU:CG	1:C:34:LYS:HB3	2.24	0.66
1:A:30:LEU:CD1	1:C:30:LEU:HB3	2.26	0.66
1:A:34:LYS:HD3	1:C:28:GLU:CA	2.26	0.66
1:C:269:THR:HG22	1:C:272:GLU:HB2	1.76	0.66
1:A:171:GLU:HA	1:A:239:GLU:HG3	1.78	0.66
1:A:266:SER:HB3	4:A:382:HOH:O	1.96	0.65
1:A:31:VAL:HG13	1:C:31:VAL:HG21	1.75	0.65
1:A:146:LYS:HD3	1:A:146:LYS:N	1.90	0.65
1:A:31:VAL:CG2	1:C:31:VAL:HG13	2.27	0.65
1:A:34:LYS:HG2	1:C:28:GLU:HB2	1.75	0.65
1:C:43:ARG:NH2	1:C:264:THR:HG21	2.12	0.64
1:A:219:PRO:HD3	2:B:47:SER:HB2	1.80	0.64
1:A:28:GLU:CA	1:A:287:HIS:CE1	2.80	0.64
1:C:35:ASP:O	1:C:39:GLN:HG2	1.97	0.64
2:B:4:PHE:N	4:B:381:HOH:O	2.31	0.64
1:A:34:LYS:HE2	1:C:30:LEU:CB	2.27	0.64
1:A:28:GLU:HA	1:A:287:HIS:CE1	2.33	0.63
2:B:8:LYS:CE	4:B:381:HOH:O	2.44	0.63
1:A:111:LYS:HG3	1:A:111:LYS:O	1.97	0.63
1:A:155:MET:HE1	1:A:192:LYS:HE2	1.80	0.63
1:C:218:GLY:N	1:C:219:PRO:HD3	2.13	0.62
1:A:34:LYS:HB3	1:C:28:GLU:CB	2.30	0.62
1:C:243:ARG:HB2	1:C:273:ARG:HH11	1.63	0.62
1:A:219:PRO:CG	2:B:47:SER:HB2	2.29	0.62
1:C:229:TRP:CZ3	1:C:285:ILE:CD1	2.83	0.61
1:A:34:LYS:HE2	1:C:30:LEU:HB2	1.83	0.61
2:D:46:GLU:HG3	2:D:47:SER:O	2.01	0.61
1:A:31:VAL:HG23	1:C:31:VAL:HA	1.66	0.61
1:A:31:VAL:CG2	1:C:31:VAL:CA	2.26	0.61
1:C:37:GLU:HG2	1:C:44:VAL:HG23	1.83	0.60
1:A:90:GLN:NE2	4:A:345:HOH:O	2.31	0.60
1:A:30:LEU:HB3	1:C:30:LEU:CD1	2.31	0.60
1:C:218:GLY:N	1:C:219:PRO:CD	2.65	0.59
1:A:280:ILE:O	1:A:284:LEU:HD12	2.01	0.59
1:A:269:THR:N	1:A:272:GLU:CG	2.61	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:ARG:HH21	1:C:264:THR:CG2	2.16	0.59
1:A:31:VAL:HG22	1:C:31:VAL:HA	0.60	0.58
1:C:39:GLN:HG3	1:C:276:GLN:HE22	1.67	0.58
1:A:35:ASP:O	1:A:39:GLN:HG3	2.03	0.58
1:A:34:LYS:CE	1:C:30:LEU:HG	2.34	0.58
1:C:269:THR:N	1:C:272:GLU:OE1	2.29	0.57
1:C:29:THR:HA	1:C:283:SER:OG	2.04	0.57
1:C:42:ALA:HB1	1:C:264:THR:O	2.05	0.57
1:A:31:VAL:CA	1:C:31:VAL:CG2	2.29	0.57
1:C:171:GLU:O	1:C:172:ALA:HB3	2.04	0.57
1:C:36:ALA:CA	1:C:276:GLN:NE2	2.57	0.56
1:A:272:GLU:O	1:A:275:ARG:HB2	2.05	0.56
1:C:208:ILE:O	1:C:212:GLU:HG3	2.06	0.56
1:A:31:VAL:CG2	1:C:31:VAL:CB	2.76	0.55
1:A:34:LYS:CB	1:C:28:GLU:CB	2.84	0.55
1:A:211:MET:O	1:A:214:ASP:HB2	2.07	0.55
1:C:36:ALA:CB	1:C:276:GLN:NE2	2.68	0.55
1:A:34:LYS:CB	1:C:28:GLU:HB2	2.37	0.55
1:A:28:GLU:HG3	1:C:34:LYS:HD3	1.88	0.55
1:A:30:LEU:HD22	1:C:30:LEU:HD12	1.81	0.54
1:A:31:VAL:HG13	1:C:31:VAL:HG11	1.80	0.54
1:A:30:LEU:N	1:C:34:LYS:CE	2.31	0.54
1:C:111:LYS:O	1:C:111:LYS:CG	2.56	0.54
1:A:30:LEU:CA	1:C:34:LYS:HE2	2.34	0.54
1:A:219:PRO:CD	2:B:47:SER:HB2	2.37	0.54
1:A:32:LYS:HE2	1:A:279:GLU:CG	2.38	0.53
2:B:98:TRP:CG	2:B:103:LYS:HD2	2.43	0.53
1:A:225:LEU:HD11	1:A:229:TRP:HB3	1.90	0.53
1:A:31:VAL:HG22	1:C:31:VAL:CG1	2.37	0.53
1:A:52:ASN:OD1	1:A:52:ASN:N	2.40	0.53
1:A:61:ARG:HD3	1:A:64:GLU:CD	2.28	0.53
1:A:225:LEU:HG	1:A:229:TRP:HB2	1.90	0.53
1:C:104:GLU:CG	4:D:349:HOH:O	2.49	0.53
1:A:61:ARG:HD3	1:A:64:GLU:OE2	2.09	0.53
1:C:37:GLU:OE2	1:C:60:PHE:HE2	1.93	0.52
1:C:43:ARG:HD2	1:C:64:GLU:OE1	2.08	0.52
1:A:171:GLU:O	1:A:172:ALA:HB3	2.09	0.52
1:A:155:MET:CE	1:A:192:LYS:HE2	2.37	0.52
1:C:269:THR:CG2	1:C:272:GLU:HB2	2.39	0.52
1:A:270:MET:HE1	4:A:350:HOH:O	2.10	0.52
1:C:243:ARG:HD3	1:C:273:ARG:HH12	1.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ALA:HB2	1:C:266:SER:HB2	1.90	0.52
1:A:28:GLU:HA	1:A:287:HIS:ND1	2.25	0.51
1:A:213:ALA:O	1:A:214:ASP:C	2.49	0.51
1:A:281:GLY:HA2	1:A:284:LEU:HD11	1.91	0.51
1:A:31:VAL:HG23	1:C:34:LYS:HD3	1.93	0.51
1:A:31:VAL:CG2	1:C:31:VAL:CG1	2.88	0.51
1:A:34:LYS:CE	1:C:30:LEU:CB	2.89	0.51
2:D:142:HIS:HB2	2:D:150:TYR:HB3	1.93	0.51
1:C:213:ALA:O	1:C:214:ASP:O	2.29	0.50
1:A:216:VAL:HG12	4:B:385:HOH:O	2.09	0.50
2:B:53:TYR:O	2:B:69:ASN:HB2	2.12	0.50
1:A:28:GLU:CG	1:C:34:LYS:CB	2.89	0.50
1:A:28:GLU:HG2	1:C:34:LYS:HB3	1.93	0.50
1:C:269:THR:CG2	1:C:272:GLU:CB	2.88	0.50
1:A:30:LEU:CG	1:C:30:LEU:CD1	2.85	0.49
1:A:269:THR:H	1:A:272:GLU:CD	2.14	0.49
1:A:284:LEU:HD22	1:A:284:LEU:C	2.32	0.49
1:A:219:PRO:HD3	2:B:47:SER:CB	2.42	0.49
2:B:124:GLU:HG3	2:B:143:LEU:HB2	1.95	0.49
1:A:30:LEU:HB2	1:C:30:LEU:CB	2.07	0.49
1:C:32:LYS:HE2	1:C:279:GLU:CG	2.38	0.49
2:D:53:TYR:O	2:D:69:ASN:HB2	2.12	0.49
1:A:111:LYS:CG	1:A:111:LYS:O	2.60	0.49
1:C:269:THR:HG22	1:C:272:GLU:HG3	1.91	0.49
2:D:124:GLU:HB2	4:D:177:HOH:O	2.12	0.49
1:A:30:LEU:CB	1:C:34:LYS:HE2	2.43	0.48
1:C:83:ARG:NH2	4:C:297:HOH:O	2.46	0.48
1:C:281:GLY:O	1:C:285:ILE:HG12	2.13	0.48
1:C:284:LEU:HD12	1:C:284:LEU:C	2.33	0.48
1:A:34:LYS:CG	1:C:28:GLU:CB	2.79	0.48
1:A:49:LEU:HD21	1:A:191:ARG:HD2	1.96	0.48
1:A:129:MET:CE	2:B:42:LEU:CD2	2.92	0.48
1:A:281:GLY:O	1:A:285:ILE:CG1	2.61	0.48
1:A:28:GLU:HG2	1:C:34:LYS:CB	2.44	0.47
1:C:32:LYS:HD2	1:C:32:LYS:HA	1.62	0.47
1:C:213:ALA:C	1:C:214:ASP:O	2.52	0.47
2:B:7:GLU:HB3	4:B:266:HOH:O	2.15	0.47
1:C:228:GLY:O	1:C:253:GLY:N	2.47	0.47
1:C:46:TYR:OH	1:C:284:LEU:HD23	2.13	0.47
1:A:208:ILE:O	1:A:212:GLU:HG3	2.15	0.47
1:C:173:ILE:HD13	1:C:173:ILE:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ILE:HB	1:A:176:ASP:HB2	1.96	0.47
1:A:129:MET:HE1	2:B:42:LEU:CD2	2.43	0.47
1:A:218:GLY:H	1:A:219:PRO:HD3	1.78	0.47
1:C:28:GLU:O	1:C:31:VAL:HB	2.15	0.47
1:C:269:THR:CG2	1:C:272:GLU:N	2.61	0.46
2:D:115:ASN:O	2:D:116:TRP:C	2.52	0.46
1:C:257:ARG:HD2	1:C:288:TRP:CH2	2.50	0.46
1:C:268:ALA:HB1	1:C:272:GLU:OE1	2.14	0.46
1:A:267:GLN:O	1:A:268:ALA:O	2.34	0.46
1:C:267:GLN:C	1:C:268:ALA:O	2.52	0.46
2:D:143:LEU:HA	2:D:147:VAL:O	2.16	0.46
1:A:162:LEU:HD12	1:A:162:LEU:HA	1.81	0.46
1:A:57:LEU:HD13	1:A:57:LEU:N	2.31	0.46
1:C:254:LYS:HE2	1:C:254:LYS:HB3	1.65	0.46
1:A:161:ARG:O	1:A:179:ASP:HA	2.16	0.46
1:C:29:THR:OG1	1:C:284:LEU:HB3	2.16	0.45
2:D:98:TRP:CE3	2:D:98:TRP:HA	2.50	0.45
2:B:8:LYS:CD	4:B:381:HOH:O	2.63	0.45
1:A:30:LEU:O	1:A:34:LYS:HD2	2.17	0.45
1:A:34:LYS:HE3	1:C:30:LEU:CA	2.34	0.45
1:C:171:GLU:O	1:C:239:GLU:HB2	2.17	0.45
1:A:211:MET:HB2	1:A:232:ALA:HB1	1.98	0.44
1:A:225:LEU:HA	1:A:226:PRO:HD3	1.83	0.44
1:C:285:ILE:HD13	1:C:285:ILE:HA	1.78	0.44
1:A:28:GLU:O	1:A:31:VAL:HB	2.17	0.44
1:A:57:LEU:CD1	1:A:57:LEU:N	2.80	0.44
1:C:267:GLN:O	1:C:268:ALA:C	2.56	0.44
1:A:30:LEU:CD1	1:C:30:LEU:CG	2.91	0.44
2:B:98:TRP:CD2	2:B:103:LYS:HD2	2.53	0.43
2:B:12:ILE:CG2	2:B:64:LEU:HD22	2.49	0.43
1:C:280:ILE:O	1:C:280:ILE:HG22	2.18	0.43
2:B:74:LYS:HB3	2:B:74:LYS:HE2	1.65	0.43
1:C:37:GLU:HG2	1:C:44:VAL:HG21	2.00	0.43
1:A:145:PRO:N	1:A:146:LYS:HD3	2.33	0.43
1:C:33:VAL:HG22	1:C:280:ILE:HD13	2.01	0.43
1:C:51:LEU:HG	1:C:195:THR:HG21	2.00	0.43
1:C:216:VAL:C	2:D:48:GLY:H	2.22	0.43
1:A:34:LYS:HD3	1:C:28:GLU:C	2.39	0.43
1:A:30:LEU:CB	1:C:30:LEU:CD1	2.97	0.43
2:B:98:TRP:HA	2:B:98:TRP:CE3	2.54	0.43
1:C:274:ASN:O	1:C:275:ARG:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LYS:HD2	1:A:32:LYS:HA	1.71	0.42
2:B:116:TRP:CZ3	2:B:119:LYS:HE2	2.54	0.42
1:C:229:TRP:HZ3	1:C:285:ILE:CD1	2.32	0.42
1:A:268:ALA:HB1	1:A:272:GLU:CG	2.42	0.42
2:B:98:TRP:CD1	2:B:103:LYS:HD2	2.54	0.42
1:C:105:TYR:CZ	2:D:50:TYR:HA	2.54	0.42
1:A:29:THR:H	1:C:34:LYS:HE3	1.79	0.42
2:B:136:PRO:HG3	4:B:194:HOH:O	2.19	0.42
1:A:285:ILE:HD13	1:A:285:ILE:HA	1.89	0.42
1:C:30:LEU:O	1:C:34:LYS:HD2	2.20	0.42
1:C:29:THR:O	1:C:33:VAL:HG23	2.20	0.42
1:C:43:ARG:NH2	1:C:264:THR:CG2	2.79	0.42
1:A:126:ALA:O	1:A:130:SER:HA	2.20	0.42
1:A:34:LYS:CE	1:C:30:LEU:HB2	2.48	0.41
1:C:93:ARG:O	1:C:118:THR:HA	2.21	0.41
1:C:225:LEU:HG	1:C:229:TRP:HB2	2.02	0.41
1:A:32:LYS:HE2	1:A:279:GLU:HG2	2.02	0.41
1:C:81:LEU:HB3	1:C:203:SER:HB3	2.02	0.41
1:A:104[B]:GLU:OE2	2:B:71:TYR:CE1	2.73	0.41
1:C:268:ALA:HB1	1:C:272:GLU:HB3	2.03	0.41
2:D:46:GLU:CG	2:D:47:SER:O	2.68	0.41
1:C:268:ALA:HB1	1:C:272:GLU:CB	2.51	0.41
1:A:34:LYS:CE	1:C:30:LEU:N	2.21	0.41
1:C:257:ARG:HB2	1:C:288:TRP:CH2	2.56	0.40
1:C:162:LEU:HD12	1:C:162:LEU:HA	1.87	0.40
1:A:61:ARG:HD3	1:A:64:GLU:OE1	2.21	0.40
1:A:220:LEU:HD23	1:A:220:LEU:HA	1.93	0.40
1:C:266:SER:OG	1:C:267:GLN:N	2.54	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	261/261 (100%)	247 (95%)	13 (5%)	1 (0%)	34	32
1	C	260/261 (100%)	244 (94%)	13 (5%)	3 (1%)	13	8
2	B	152/156 (97%)	150 (99%)	2 (1%)	0	100	100
2	D	155/156 (99%)	153 (99%)	1 (1%)	1 (1%)	25	21
All	All	828/834 (99%)	794 (96%)	29 (4%)	5 (1%)	25	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	ALA
1	C	268	ALA
1	C	275	ARG
2	D	79	SER
1	C	52	ASN

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	218/216 (101%)	208 (95%)	10 (5%)	27	26
1	C	217/216 (100%)	207 (95%)	10 (5%)	27	26
2	B	124/125 (99%)	123 (99%)	1 (1%)	81	86
2	D	126/125 (101%)	122 (97%)	4 (3%)	39	41
All	All	685/682 (100%)	660 (96%)	25 (4%)	34	36

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	52	ASN
1	A	57	LEU
1	A	72	PHE
1	A	146	LYS
1	A	173	ILE

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Mol	Chain	Res	Type
1	A	239	GLU
1	A	272	GLU
1	A	279	GLU
1	A	284	LEU
2	B	134	LEU
1	C	32	LYS
1	C	43	ARG
1	C	52	ASN
1	C	72	PHE
1	C	110	GLU
1	C	130	SER
1	C	175	ASN
1	C	231	ILE
1	C	264	THR
1	C	279	GLU
2	D	2	SER
2	D	13	GLN
2	D	23	GLU
2	D	47	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	287	HIS
2	B	84	HIS
2	B	109	GLN
1	C	158	HIS
1	C	276	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

4 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	$\# Z > 2$
3	PO4	B	158	-	4,4,4	0.65	0	6,6,6	0.88	0
3	PO4	C	2	-	4,4,4	0.54	0	6,6,6	0.55	0
3	PO4	D	158	-	4,4,4	0.18	0	6,6,6	1.54	2 (33%)
3	PO4	B	1	-	4,4,4	0.32	0	6,6,6	1.21	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	158	PO4	O3-P-O2	2.37	115.58	107.97
3	D	158	PO4	O4-P-O2	-2.33	100.50	107.97

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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	261/261 (100%)	-0.23	7 (2%) 54 60	12, 25, 57, 67	0
1	C	261/261 (100%)	-0.07	18 (6%) 16 21	12, 25, 59, 70	0
2	B	154/156 (98%)	-0.60	0 100 100	11, 18, 28, 41	0
2	D	156/156 (100%)	-0.58	0 100 100	11, 18, 28, 47	0
All	All	832/834 (99%)	-0.31	25 (3%) 50 56	11, 22, 56, 70	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	31	VAL	5.8
1	A	36	ALA	4.6
1	C	40	LEU	4.3
1	C	33	VAL	4.0
1	C	218	GLY	4.0
1	C	217	ALA	3.9
1	C	275	ARG	3.3
1	C	285	ILE	3.3
1	C	219	PRO	3.2
1	C	216	VAL	3.1
1	C	42	ALA	3.0
1	A	31	VAL	3.0
1	C	221	LEU	3.0
1	A	38	ASP	2.9
1	C	28	GLU	2.9
1	C	36	ALA	2.7
1	A	40	LEU	2.6
1	C	225	LEU	2.6
1	C	38	ASP	2.5
1	C	30	LEU	2.4
1	C	220	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	220	LEU	2.3
1	A	39	GLN	2.3
1	C	270	MET	2.0
1	A	275	ARG	2.0

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PO4	B	158	5/5	0.93	0.14	65,69,70,71	0
3	PO4	C	2	5/5	0.95	0.08	51,52,56,56	0
3	PO4	D	158	5/5	0.96	0.09	23,27,30,32	0
3	PO4	B	1	5/5	0.97	0.08	29,29,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.