Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2025 – 03:15 PM EDT

PDB ID	:	3GMW / pdb_00003gmw
Title	:	Crystal Structure of Beta-Lactamse 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

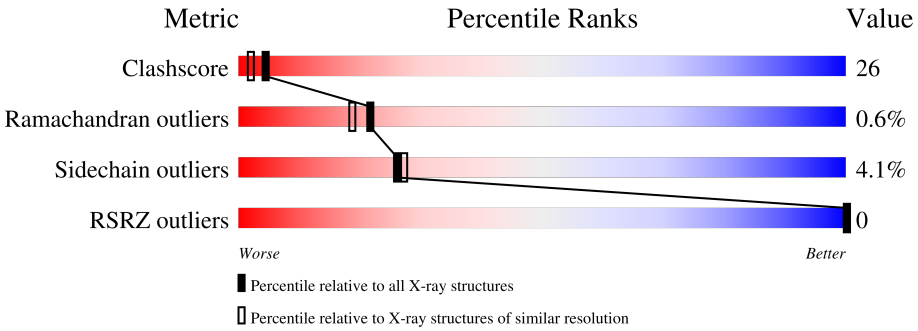
MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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	180529	6893 (2.10-2.10)
Ramachandran outliers	177936	6839 (2.10-2.10)
Sidechain outliers	177891	6840 (2.10-2.10)
RSRZ outliers	164620	6234 (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 of 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	261	67% 26% 6%
1	C	261	70% 26% •
2	B	156	80% 17% ••
2	D	156	88% 10% •

2 Entry composition

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.

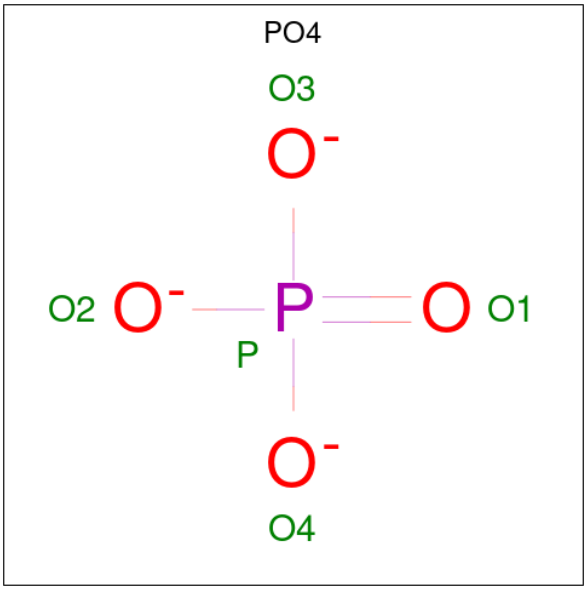
- Molecule 1 is a protein called B-lactamase.

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

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

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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 4 is water.

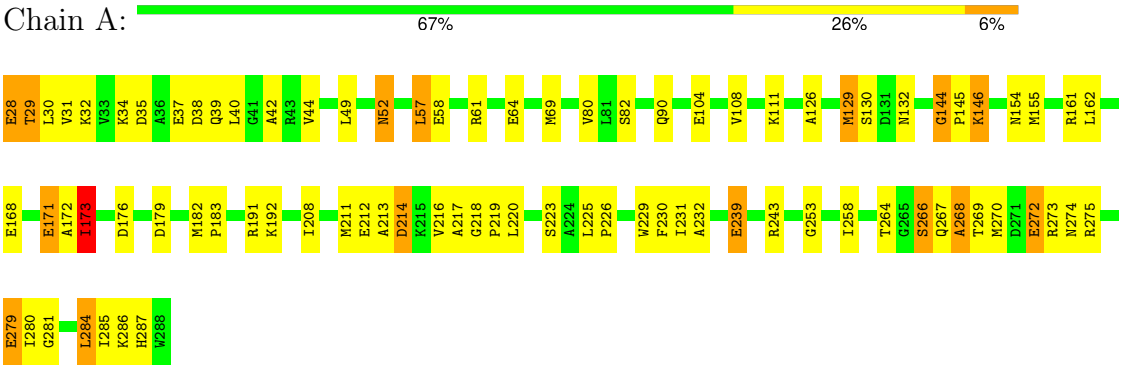
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	75	Total O 75 75	0	0
4	B	106	Total O 106 106	0	0
4	C	79	Total O 79 79	0	0
4	D	112	Total O 112 112	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

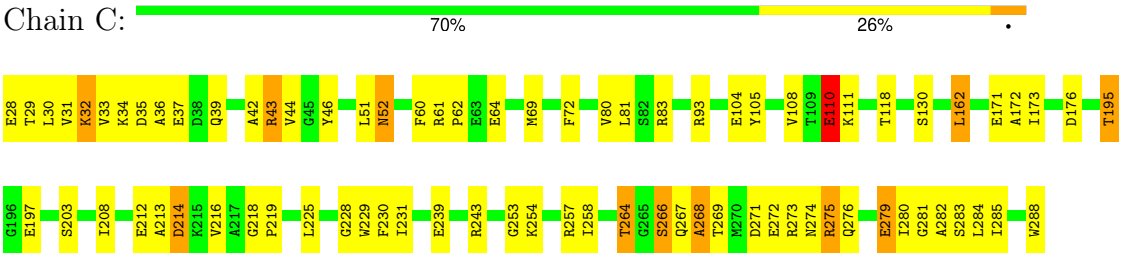
• Molecule 1: B-lactamase

Chain A:



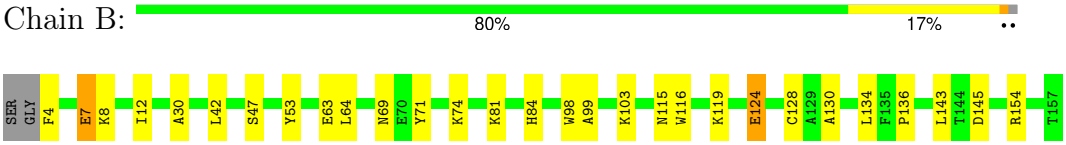
• Molecule 1: B-lactamase

Chain C:



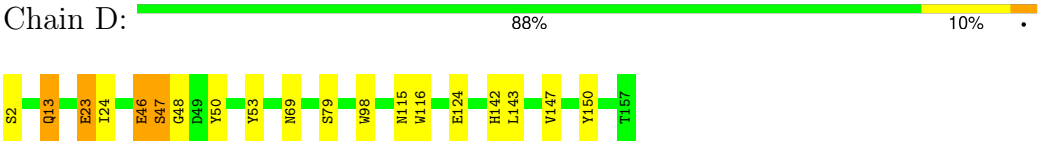
• Molecule 2: Beta-lactamase inhibitory protein BLIP-I

Chain B:



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

Chain D:



4 Data and refinement statistics (i)

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 25.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	95.0 (25.00-2.10) 94.4 (25.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [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)	0.35 , 22.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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 $< |L| >$, $< L^2 >$ 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: 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	1.19	0/2061	1.25	15/2789 (0.5%)
1	C	1.18	1/2055 (0.0%)	1.22	9/2781 (0.3%)
2	B	1.41	4/1241 (0.3%)	1.26	3/1683 (0.2%)
2	D	1.41	2/1260 (0.2%)	1.23	0/1708
All	All	1.27	7/6617 (0.1%)	1.24	27/8961 (0.3%)

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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	145	ASP	CA-C	5.81	1.60	1.53
2	D	23	GLU	C-O	-5.65	1.17	1.24
1	C	258	ILE	CA-CB	-5.27	1.48	1.54
2	B	63	GLU	N-CA	5.27	1.52	1.46
2	B	128	CYS	C-O	-5.15	1.18	1.24
2	B	30	ALA	CA-CB	-5.12	1.46	1.54
2	D	24	ILE	CA-CB	-5.06	1.48	1.54

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	197	GLU	N-CA-C	-7.38	103.84	112.92
1	A	29	THR	N-CA-C	6.81	118.35	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	214	ASP	N-CA-C	-6.25	101.60	110.35
1	C	282	ALA	N-CA-C	-5.79	104.34	111.75
1	C	266	SER	N-CA-C	5.70	118.05	110.53
1	A	108	VAL	CB-CA-C	-5.69	105.01	111.55
1	A	258	ILE	CB-CA-C	-5.66	102.40	110.83
1	C	108	VAL	CB-CA-C	-5.66	105.04	111.55
1	A	266	SER	N-CA-C	5.63	118.44	110.50
1	C	80	VAL	N-CA-C	5.60	115.80	110.42
1	A	82	SER	N-CA-C	-5.56	105.30	111.36
2	B	130	ALA	N-CA-C	-5.48	106.59	113.28
1	A	171	GLU	N-CA-C	5.43	116.88	111.07
1	C	214	ASP	N-CA-C	-5.43	102.75	110.35
1	A	168	GLU	N-CA-C	5.41	117.94	111.71
1	C	195	THR	N-CA-C	-5.40	107.70	114.56
1	A	132	ASN	N-CA-C	5.32	116.76	111.07
2	B	99	ALA	N-CA-C	-5.32	106.30	112.89
1	A	80	VAL	N-CA-C	5.30	115.51	110.42
1	A	173	ILE	CA-C-N	-5.23	114.37	119.76
1	A	173	ILE	C-N-CA	-5.23	114.37	119.76
1	C	110	GLU	CA-CB-CG	5.17	124.45	114.10
2	B	7	GLU	CB-CG-CD	5.12	121.30	112.60
1	A	144	GLY	CA-C-N	5.05	125.08	119.32
1	A	144	GLY	C-N-CA	5.05	125.08	119.32
1	A	129	MET	CB-CG-SD	-5.05	97.55	112.70
1	C	162	LEU	N-CA-C	-5.04	101.48	109.59

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	198	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2020	0	2037	199	0
2	B	1205	0	1111	31	0
2	D	1221	0	1125	13	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	333	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 26.

All (333) 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
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:155:MET:HE2	1:A:192:LYS:HE3	1.22	1.18
1:A:30:LEU:HD22	1:C:30:LEU:HD13	1.27	1.16
1:A:31:VAL:CB	1:C:31:VAL:HG22	1.74	1.14
1:C:269:THR:HG23	1:C:272:GLU:H	0.98	1.14
1:A:146:LYS:H	1:A:146:LYS:HD3	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:H	1:A:146:LYS:HD2	1.04	1.09
1:A:31:VAL:HG13	1:C:31:VAL:CG1	1.85	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:30:LEU:HD22	1:C:30:LEU:CD1	1.85	1.05
1:A:34:LYS:CD	1:C:28:GLU:HB2	1.87	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
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:155:MET:HE2	1:A:192:LYS:CE	1.99	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:28:GLU:N	1:A:287:HIS:CE1	2.40	0.89
1:A:220:LEU:O	1:A:223:SER:HB3	1.72	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:30:LEU:CD1	1:C:30:LEU:HD13	2.04	0.86
1:A:34:LYS:CB	1:C:28:GLU:CG	2.51	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:129:MET:HE1	2:B:42:LEU:HD23	1.59	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
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:213:ALA:O	1:C:214:ASP:C	2.29	0.75
1:C:28:GLU:N	1:C:31:VAL:HG21	2.01	0.75
1:C:269:THR:HG22	1:C:272:GLU:CB	2.17	0.75
1:A:31:VAL:HG11	1:C:31:VAL:HG13	1.66	0.75
1:C:111:LYS:O	1:C:111:LYS:HG2	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:31:VAL:CB	1:C:31:VAL:CG2	2.62	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:THR:N	1:A:272:GLU:HG3	2.03	0.73
1:C:269:THR:HG22	1:C:272:GLU:CD	2.12	0.73
2:B:124:GLU:OE2	4:B:210:HOH:O	2.06	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: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: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
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:A:155:MET:HE1	1:A:192:LYS:CE	2.24	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:31:VAL:CG2	1:C:31:VAL:HG13	2.27	0.65
1:A:146:LYS:HD3	1:A:146:LYS:N	1.90	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:28:GLU:CA	1:A:287:HIS:CE1	2.80	0.64
1:A:219:PRO:HD3	2:B:47:SER:HB2	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:218:GLY:N	1:C:219:PRO:HD3	2.13	0.62
1:A:111:LYS:O	1:A:111:LYS:HG3	1.97	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
1:C:43:ARG:HH21	1:C:264:THR:CG2	2.16	0.59
1:A:61:ARG:HD3	1:A:64:GLU:CD	2.28	0.58
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:A:155:MET:HE1	1:A:192:LYS:HE2	1.85	0.57
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:A:213:ALA:O	1:A:214:ASP:C	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LEU:N	1:C:34:LYS:CE	2.31	0.54
1:A:31:VAL:HG13	1:C:31:VAL:HG11	1.80	0.54
1:A:30:LEU:CA	1:C:34:LYS:HE2	2.34	0.54
1:C:111:LYS:O	1:C:111:LYS:CG	2.56	0.54
1:A:269:THR:H	1:A:272:GLU:CD	2.14	0.54
1:A:284:LEU:C	1:A:284:LEU:HD22	2.32	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:31:VAL:HG22	1:C:31:VAL:CG1	2.37	0.53
1:A:225:LEU:HD11	1:A:229:TRP:HB3	1.90	0.53
1:A:52:ASN:OD1	1:A:52:ASN:N	2.40	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:C:284:LEU:C	1:C:284:LEU:HD12	2.33	0.53
1:A:270:MET:HE1	4:A:350:HOH:O	2.09	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:C:213:ALA:C	1:C:214:ASP:O	2.52	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:C:42:ALA:HB2	1:C:266:SER:HB2	1.90	0.52
1:C:243:ARG:HD3	1:C:273:ARG:HH12	1.72	0.52
1:A:28:GLU:HA	1:A:287:HIS:ND1	2.25	0.51
2:D:115:ASN:O	2:D:116:TRP:C	2.52	0.51
1:A:281:GLY:HA2	1:A:284:LEU:HD11	1.91	0.51
1:A:269:THR:HG1	1:A:272:GLU:HG2	1.74	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
1:C:267:GLN:C	1:C:268:ALA:O	2.52	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
1:A:28:GLU:CG	1:C:34:LYS:CB	2.89	0.50
2:B:53:TYR:O	2:B:69:ASN:HB2	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:PRO:HD3	2:B:47:SER:CB	2.42	0.49
1:A:30:LEU:HB2	1:C:30:LEU:CB	2.07	0.49
2:B:124:GLU:HG3	2:B:143:LEU:HB2	1.95	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:O	1:A:111:LYS:CG	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:267:GLN:O	1:C:268:ALA:C	2.56	0.48
1:C:281:GLY:O	1:C:285:ILE:HG12	2.13	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:C:216:VAL:C	2:D:48:GLY:H	2.22	0.48
1:A:28:GLU:HG2	1:C:34:LYS:CB	2.44	0.47
1:A:34:LYS:HD3	1:C:28:GLU:C	2.39	0.47
1:C:32:LYS:HA	1:C:32:LYS:HD2	1.62	0.47
1:C:274:ASN:O	1:C:275:ARG:C	2.56	0.47
1:A:69:MET:HE1	1:A:243:ARG:C	2.39	0.47
2:B:7:GLU:HB3	4:B:266:HOH:O	2.15	0.47
1:C:46:TYR:OH	1:C:284:LEU:HD23	2.13	0.47
1:C:228:GLY:O	1:C:253:GLY:N	2.47	0.47
1:A:208:ILE:O	1:A:212:GLU:HG3	2.15	0.47
1:C:173:ILE:N	1:C:173:ILE:HD13	2.28	0.47
1:A:173:ILE:HB	1:A:176:ASP:HB2	1.96	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
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
2:D:143:LEU:HA	2:D:147:VAL:O	2.16	0.46
1:A:57:LEU:N	1:A:57:LEU:HD13	2.31	0.46
1:A:162:LEU:HD12	1:A:162:LEU:HA	1.81	0.46
1:C:254:LYS:HB3	1:C:254:LYS:HE2	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:HA	2:D:98:TRP:CE3	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:230:PHE:HB2	1:A:253:GLY:C	2.43	0.44
1:A:57:LEU:N	1:A:57:LEU:CD1	2.80	0.44
1:A:30:LEU:CD1	1:C:30:LEU:CG	2.91	0.44
2:B:115:ASN:O	2:B:116:TRP:C	2.61	0.44
1:A:213:ALA:C	1:A:214:ASP:O	2.60	0.43
1:A:273:ARG:O	1:A:274:ASN:C	2.60	0.43
2:B:98:TRP:CD2	2:B:103:LYS:HD2	2.53	0.43
1:A:144:GLY:C	1:A:146:LYS:HD3	2.44	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: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: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
1:A:29:THR:H	1:C:34:LYS:HE3	1.79	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
2:B:136:PRO:HG3	4:B:194:HOH:O	2.19	0.42
1:A:28:GLU:CD	1:C:34:LYS:HB3	2.44	0.42
1:A:285:ILE:HD13	1:A:285:ILE:HA	1.89	0.42
1:C:29:THR:O	1:C:33:VAL:HG23	2.20	0.42
1:C:30:LEU:O	1:C:34:LYS:HD2	2.20	0.42
1:C:43:ARG:NH2	1:C:264:THR:CG2	2.79	0.42
1:C:212:GLU:CD	1:C:230:PHE:CE2	2.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:69:MET:HE1	1:C:243:ARG:C	2.46	0.41
1:C:81:LEU:HB3	1:C:203:SER:HB3	2.02	0.41
1:C:61[A]:ARG:HD3	1:C:64:GLU:CD	2.45	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
1:C:281:GLY:C	1:C:283:SER:N	2.77	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
2:D:53:TYR:CD1	2:D:53:TYR:C	2.99	0.41
1:A:217:ALA:C	1:A:219:PRO:CD	2.94	0.40
1:C:257:ARG:HB2	1:C:288:TRP:CH2	2.56	0.40
1:C:110:GLU:CD	1:C:110:GLU:C	2.89	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:182:MET:O	1:A:183:PRO:C	2.62	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%)	30 29
1	C	260/261 (100%)	244 (94%)	13 (5%)	3 (1%)	11 7
2	B	152/156 (97%)	150 (99%)	2 (1%)	0	100 100
2	D	155/156 (99%)	153 (99%)	1 (1%)	1 (1%)	22 19

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	828/834 (99%)	794 (96%)	29 (4%)	5 (1%)	22 19

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%)	206 (94%)	12 (6%)	18 16
1	C	217/216 (100%)	208 (96%)	9 (4%)	26 27
2	B	124/125 (99%)	122 (98%)	2 (2%)	58 65
2	D	126/125 (101%)	121 (96%)	5 (4%)	27 28
All	All	685/682 (100%)	657 (96%)	28 (4%)	26 27

All (28) 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	58	GLU
1	A	146	LYS
1	A	173	ILE
1	A	231	ILE
1	A	239	GLU
1	A	272	GLU
1	A	279	GLU

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Mol	Chain	Res	Type
1	A	284	LEU
1	A	286	LYS
2	B	124	GLU
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	231	ILE
1	C	264	THR
1	C	279	GLU
2	D	2	SER
2	D	13	GLN
2	D	23	GLU
2	D	46	GLU
2	D	47	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	100	ASN
1	A	206	GLN
1	A	287	HIS
2	B	84	HIS
2	B	109	GLN
1	C	99	GLN
1	C	100	ASN
1	C	153	HIS
1	C	206	GLN
1	C	276	GLN
2	D	13	GLN

5.3.3 RNA

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 oligosaccharides 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	1	-	4,4,4	0.37	0	6,6,6	1.27	0
3	PO4	B	158	-	4,4,4	0.69	0	6,6,6	0.92	0
3	PO4	C	2	-	4,4,4	0.58	0	6,6,6	0.58	0
3	PO4	D	158	-	4,4,4	0.22	0	6,6,6	1.59	2 (33%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	158	PO4	O3-P-O2	2.46	115.58	107.91
3	D	158	PO4	O4-P-O2	-2.38	100.50	107.91

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, 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	261/261 (100%)	-1.40	0	100	100	10, 25, 57, 67	2 (0%)
1	C	261/261 (100%)	-1.37	0	100	100	12, 25, 59, 70	1 (0%)
2	B	154/156 (98%)	-1.54	0	100	100	11, 18, 28, 41	0
2	D	156/156 (100%)	-1.51	0	100	100	11, 18, 28, 47	1 (0%)
All	All	832/834 (99%)	-1.44	0	100	100	10, 22, 56, 70	4 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	PO4	B	158	5/5	0.97	0.05	65,69,70,71	0
3	PO4	B	1	5/5	0.99	0.05	29,29,35,35	0
3	PO4	C	2	5/5	0.99	0.04	51,52,56,56	0
3	PO4	D	158	5/5	0.99	0.05	23,27,30,32	0

6.5 Other polymers (i)

There are no such residues in this entry.