



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 05:56 PM EDT

PDB ID : 3K17  
Title : Crystal structure of a Lin0012 protein from *Listeria innocua*  
Authors : Palani, K.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center  
for Structural Genomics (NYSGXRC)  
Deposited on : 2009-09-25  
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](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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

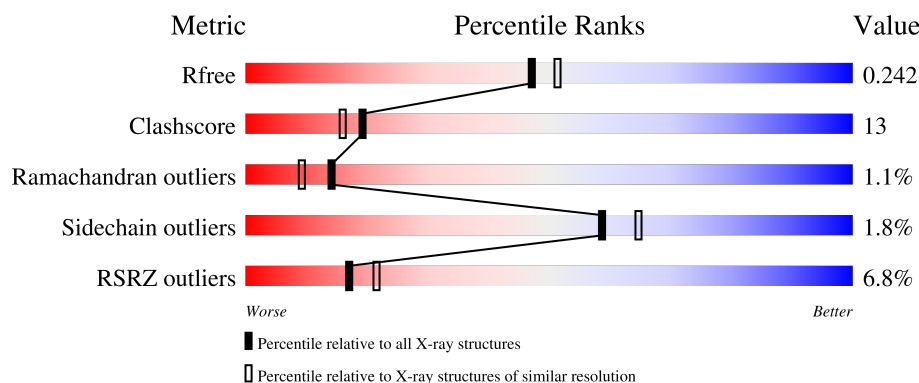
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	130704	5197 (2.10-2.10)
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 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	365	<div> <div>0%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>..</div> </div> </div>
1	B	365	<div> <div>6%</div> <div> <div></div> <div>69%</div> <div>26%</div> <div>..</div> </div> </div>
1	C	365	<div> <div>3%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>..</div> </div> </div>
1	D	365	<div> <div>16%</div> <div> <div></div> <div>69%</div> <div>25%</div> <div>..</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11491 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 Lin0012 protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	Se	0	0	0
			2774	1776	459	528	3	8			
1	B	355	Total	C	N	O	S	Se	0	0	0
			2774	1776	459	528	3	8			
1	C	355	Total	C	N	O	S	Se	0	0	0
			2774	1776	459	528	3	8			
1	D	355	Total	C	N	O	S	Se	0	0	0
			2774	1776	459	528	3	8			

There are 40 discrepancies between the modelled and reference sequences:

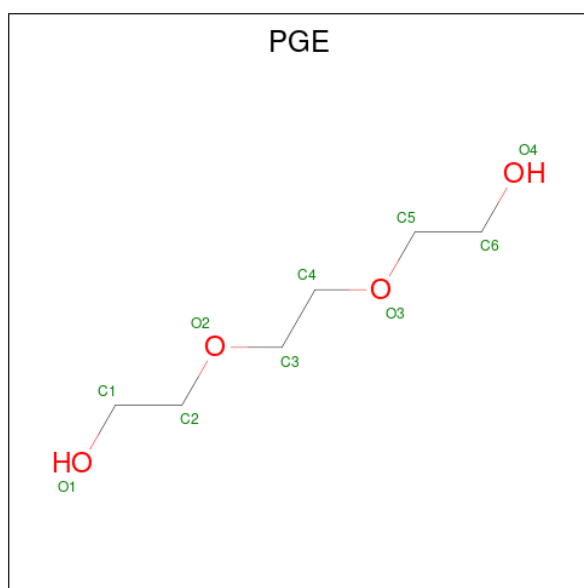
Chain	Residue	Modelled	Actual	Comment	Reference
A	3	MSE	-	expression tag	UNP Q92FU1
A	4	SER	-	expression tag	UNP Q92FU1
A	5	LEU	-	expression tag	UNP Q92FU1
A	361	GLY	-	expression tag	UNP Q92FU1
A	362	HIS	-	expression tag	UNP Q92FU1
A	363	HIS	-	expression tag	UNP Q92FU1
A	364	HIS	-	expression tag	UNP Q92FU1
A	365	HIS	-	expression tag	UNP Q92FU1
A	366	HIS	-	expression tag	UNP Q92FU1
A	367	HIS	-	expression tag	UNP Q92FU1
B	3	MSE	-	expression tag	UNP Q92FU1
B	4	SER	-	expression tag	UNP Q92FU1
B	5	LEU	-	expression tag	UNP Q92FU1
B	361	GLY	-	expression tag	UNP Q92FU1
B	362	HIS	-	expression tag	UNP Q92FU1
B	363	HIS	-	expression tag	UNP Q92FU1
B	364	HIS	-	expression tag	UNP Q92FU1
B	365	HIS	-	expression tag	UNP Q92FU1
B	366	HIS	-	expression tag	UNP Q92FU1
B	367	HIS	-	expression tag	UNP Q92FU1
C	3	MSE	-	expression tag	UNP Q92FU1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	4	SER	-	expression tag	UNP Q92FU1
C	5	LEU	-	expression tag	UNP Q92FU1
C	361	GLY	-	expression tag	UNP Q92FU1
C	362	HIS	-	expression tag	UNP Q92FU1
C	363	HIS	-	expression tag	UNP Q92FU1
C	364	HIS	-	expression tag	UNP Q92FU1
C	365	HIS	-	expression tag	UNP Q92FU1
C	366	HIS	-	expression tag	UNP Q92FU1
C	367	HIS	-	expression tag	UNP Q92FU1
D	3	MSE	-	expression tag	UNP Q92FU1
D	4	SER	-	expression tag	UNP Q92FU1
D	5	LEU	-	expression tag	UNP Q92FU1
D	361	GLY	-	expression tag	UNP Q92FU1
D	362	HIS	-	expression tag	UNP Q92FU1
D	363	HIS	-	expression tag	UNP Q92FU1
D	364	HIS	-	expression tag	UNP Q92FU1
D	365	HIS	-	expression tag	UNP Q92FU1
D	366	HIS	-	expression tag	UNP Q92FU1
D	367	HIS	-	expression tag	UNP Q92FU1

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		

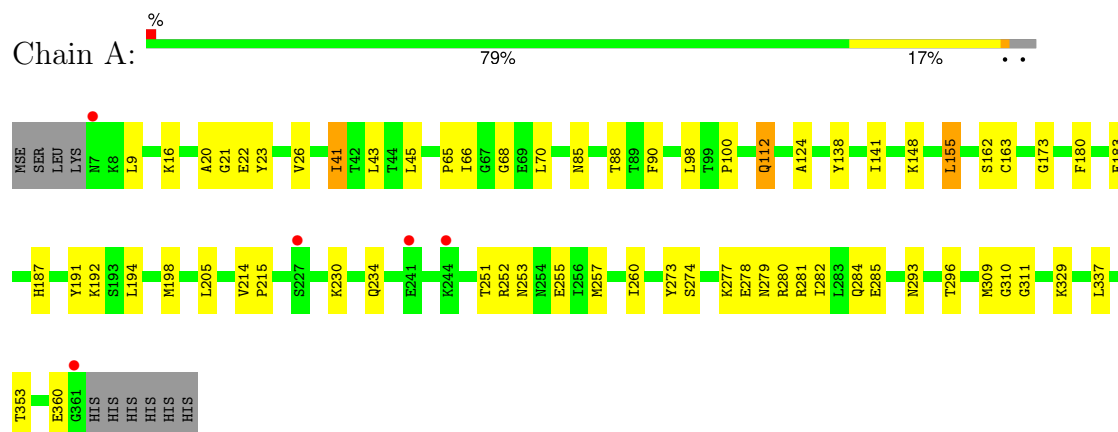
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	128	Total 128	O 128	0	0
3	B	69	Total 69	O 69	0	0
3	C	124	Total 124	O 124	0	0
3	D	64	Total 64	O 64	0	0

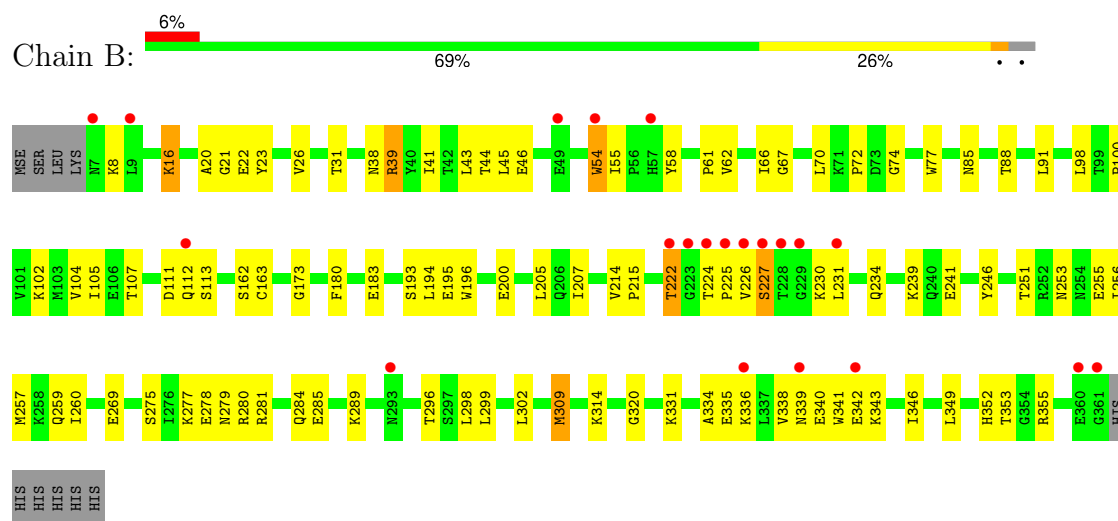
### 3 Residue-property plots [i](#)

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.

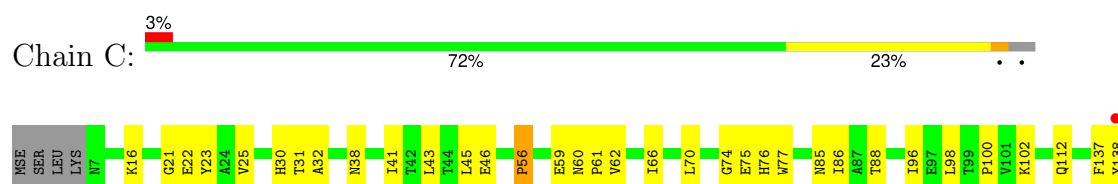
#### • Molecule 1: Lin0012 protein

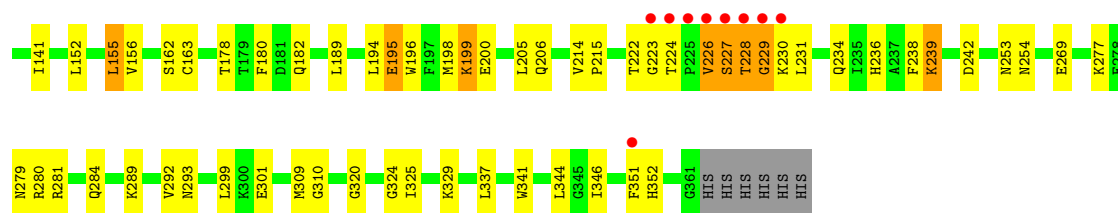


#### • Molecule 1: Lin0012 protein

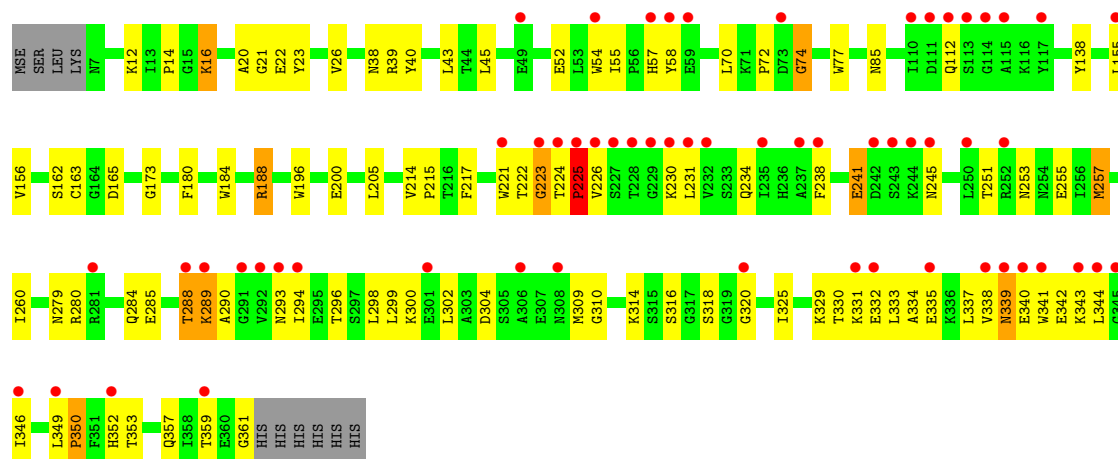


#### • Molecule 1: Lin0012 protein





● Molecule 1: Lin0012 protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.97Å 122.36Å 138.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.06 – 2.10 43.06 – 2.09	Depositor EDS
% Data completeness (in resolution range)	96.3 (43.06-2.10) 95.8 (43.06-2.09)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.00 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.223 , 0.252 0.215 , 0.242	Depositor DCC
$R_{free}$ test set	5099 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.9	Xtriage
Anisotropy	0.285	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11491	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.73% 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: PGE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.34	0/2829	0.59	1/3818 (0.0%)
1	B	0.30	0/2829	0.55	0/3818
1	C	0.34	0/2829	0.62	2/3818 (0.1%)
1	D	0.29	0/2829	0.55	0/3818
All	All	0.32	0/11316	0.58	3/15272 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	41	ILE	N-CA-C	-5.52	96.11	111.00
1	A	41	ILE	N-CA-C	-5.30	96.69	111.00
1	C	324	GLY	N-CA-C	-5.19	100.11	113.10

There are no chirality outliers.

There are no planarity outliers.

### 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	2774	0	2762	50	0
1	B	2774	0	2762	86	0
1	C	2774	0	2762	71	0
1	D	2774	0	2762	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	10	0	14	4	0
3	A	128	0	0	0	0
3	B	69	0	0	1	0
3	C	124	0	0	2	0
3	D	64	0	0	0	0
All	All	11491	0	11062	285	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 13.

All (285) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:VAL:HG22	1:C:227:SER:H	1.20	1.01
1:D:245:ASN:HD22	1:D:289:LYS:HD2	1.22	1.01
1:D:257:MSE:HE2	1:D:260:ILE:HG21	1.41	0.98
1:C:21:GLY:HA2	1:C:253:ASN:HD21	1.37	0.90
1:A:70:LEU:H	1:A:85:ASN:HD21	1.18	0.88
1:C:70:LEU:H	1:C:85:ASN:HD21	1.23	0.84
1:B:70:LEU:H	1:B:85:ASN:HD21	1.25	0.82
1:C:21:GLY:H	1:C:279:ASN:HD21	1.26	0.81
1:D:245:ASN:ND2	1:D:289:LYS:HD2	1.95	0.81
1:D:70:LEU:H	1:D:85:ASN:HD21	1.28	0.81
1:B:331:LYS:O	1:B:335:GLU:HG3	1.83	0.78
1:A:9:LEU:HD13	1:A:360:GLU:HG2	1.66	0.77
1:A:20:ALA:HB1	1:A:257:MSE:HE1	1.66	0.76
1:A:41:ILE:HD12	1:A:124:ALA:HB3	1.67	0.75
1:D:39:ARG:HH21	1:D:349:LEU:HB3	1.49	0.75
1:D:296:THR:H	1:D:299:LEU:HD12	1.50	0.75
1:C:226:VAL:HG22	1:C:227:SER:N	2.00	0.75
1:D:184:TRP:O	1:D:188:ARG:HD2	1.86	0.75
1:B:21:GLY:HA2	1:B:253:ASN:HD21	1.51	0.74
1:A:21:GLY:HA2	1:A:253:ASN:HD21	1.52	0.74
1:A:21:GLY:H	1:A:279:ASN:HD21	1.36	0.73
1:D:257:MSE:HE2	1:D:260:ILE:CG2	2.18	0.73
1:D:21:GLY:HA2	1:D:253:ASN:HD21	1.54	0.72
1:D:257:MSE:HA	1:D:257:MSE:HE3	1.69	0.72
1:C:289:LYS:HE3	3:C:427:HOH:O	1.88	0.72
1:C:277:LYS:O	1:C:281:ARG:HG2	1.91	0.71
1:C:309:MSE:HE3	1:C:337:LEU:HA	1.72	0.70
1:A:277:LYS:O	1:A:281:ARG:HG2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:GLY:H	1:B:279:ASN:HD21	1.38	0.70
1:A:310:GLY:O	1:A:329:LYS:HE3	1.92	0.69
1:D:257:MSE:HA	1:D:257:MSE:CE	2.23	0.68
1:A:194:LEU:H	2:A:1:PGE:H22	1.59	0.67
1:C:178:THR:HB	1:C:206:GLN:HB2	1.77	0.67
1:A:194:LEU:N	2:A:1:PGE:H22	2.10	0.67
1:C:30:HIS:CD2	1:C:254:ASN:HD21	2.13	0.67
1:D:279:ASN:ND2	1:D:314:LYS:HE3	2.08	0.67
1:A:230:LYS:HD2	1:B:241:GLU:OE2	1.96	0.66
1:A:281:ARG:O	1:A:285:GLU:HG2	1.96	0.66
1:B:8:LYS:HB3	1:B:46:GLU:HB3	1.79	0.65
1:A:230:LYS:O	1:A:234:GLN:HG3	1.95	0.65
1:C:222:THR:O	1:C:224:THR:N	2.31	0.63
1:C:196:TRP:CH2	1:C:200:GLU:HG2	2.34	0.63
1:A:183:GLU:HG2	1:A:187:HIS:CE1	2.34	0.63
1:B:340:GLU:HA	1:B:343:LYS:HE2	1.82	0.62
1:A:41:ILE:HD12	1:A:124:ALA:CB	2.29	0.62
1:D:329:LYS:HB2	1:D:333:LEU:HD12	1.81	0.62
1:B:309:MSE:HE3	1:B:309:MSE:HA	1.82	0.62
1:C:155:LEU:HD12	1:C:155:LEU:C	2.21	0.61
1:D:196:TRP:CH2	1:D:200:GLU:HG2	2.36	0.61
1:B:173:GLY:HA2	1:B:353:THR:CG2	2.30	0.61
1:A:173:GLY:HA2	1:A:353:THR:CG2	2.30	0.60
1:B:16:LYS:HD2	1:B:16:LYS:C	2.22	0.60
1:D:52:GLU:CD	1:D:54:TRP:HE1	2.05	0.60
1:D:180:PHE:HB3	1:D:205:LEU:HB2	1.84	0.60
1:D:334:ALA:O	1:D:338:VAL:HG23	2.00	0.60
1:D:23:TYR:O	1:D:26:VAL:HG22	2.02	0.59
1:A:88:THR:HG23	1:A:98:LEU:CD1	2.32	0.59
1:D:332:GLU:CD	1:D:332:GLU:H	2.05	0.59
1:B:277:LYS:O	1:B:281:ARG:HG2	2.01	0.58
1:C:195:GLU:O	1:C:199:LYS:HD2	2.02	0.58
1:B:38:ASN:HB3	1:B:352:HIS:HB2	1.85	0.58
1:B:336:LYS:O	1:B:339:ASN:HB3	2.03	0.58
1:B:180:PHE:HB3	1:B:205:LEU:HB2	1.86	0.58
1:A:280:ARG:O	1:A:284:GLN:HG3	2.03	0.58
1:B:54:TRP:CZ3	1:B:102:LYS:HE3	2.39	0.58
1:D:285:GLU:O	1:D:289:LYS:HG2	2.04	0.58
1:C:66:ILE:HD13	1:C:100:PRO:HD3	1.86	0.57
1:B:23:TYR:O	1:B:26:VAL:HG22	2.04	0.57
1:B:222:THR:CG2	1:B:299:LEU:HD23	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ILE:HG12	1:B:275:SER:HB3	1.86	0.57
1:C:155:LEU:HD12	1:C:156:VAL:N	2.19	0.57
1:D:221:TRP:CE2	1:D:223:GLY:HA2	2.38	0.57
1:B:285:GLU:HG3	1:B:289:LYS:HE3	1.86	0.57
1:D:309:MSE:HE3	1:D:337:LEU:N	2.20	0.57
1:B:162:SER:O	1:B:163:CYS:HB2	2.05	0.57
1:B:39:ARG:HH12	1:B:349:LEU:HD22	1.69	0.57
1:B:222:THR:HG21	1:B:299:LEU:HD23	1.87	0.56
1:D:20:ALA:HB1	1:D:257:MSE:HE1	1.88	0.56
1:B:230:LYS:HB2	1:B:230:LYS:NZ	2.20	0.56
1:B:214:VAL:HB	1:B:215:PRO:HD3	1.85	0.56
1:C:226:VAL:CG2	1:C:227:SER:H	1.98	0.56
1:A:22:GLU:O	1:A:23:TYR:HB2	2.05	0.56
1:D:359:THR:HG22	1:D:361:GLY:H	1.69	0.56
1:A:162:SER:O	1:A:163:CYS:HB2	2.06	0.56
1:D:162:SER:O	1:D:163:CYS:HB2	2.06	0.56
1:D:280:ARG:O	1:D:284:GLN:HG3	2.06	0.56
1:C:231:LEU:HD23	1:C:292:VAL:HG21	1.88	0.55
1:D:74:GLY:HA3	1:D:77:TRP:HD1	1.70	0.55
1:D:55:ILE:HD11	1:D:58:TYR:CD2	2.41	0.55
1:A:138:TYR:CD2	1:A:141:ILE:HB	2.42	0.55
1:C:88:THR:HG23	1:C:98:LEU:CD1	2.36	0.55
1:B:20:ALA:HB1	1:B:279:ASN:HD22	1.72	0.54
1:D:38:ASN:HB3	1:D:352:HIS:HB2	1.90	0.54
1:B:31:THR:O	1:B:257:MSE:HG2	2.06	0.54
1:C:194:LEU:O	1:C:198:MSE:HG2	2.08	0.54
1:C:228:THR:HG23	1:C:229:GLY:N	2.23	0.54
1:C:152:LEU:O	1:C:156:VAL:HG13	2.08	0.54
1:D:16:LYS:HE2	1:D:16:LYS:C	2.28	0.54
1:B:111:ASP:C	1:B:113:SER:H	2.10	0.54
1:C:86:ILE:HG23	1:C:194:LEU:HD21	1.90	0.54
1:B:302:LEU:C	1:B:302:LEU:HD23	2.28	0.54
1:B:39:ARG:HG2	1:B:39:ARG:HH11	1.72	0.53
1:C:180:PHE:CE1	1:C:182:GLN:HG2	2.42	0.53
1:B:302:LEU:HB2	1:B:346:ILE:HD13	1.91	0.53
1:A:112:GLN:CD	1:A:112:GLN:H	2.11	0.53
1:B:70:LEU:HG	1:B:72:PRO:HD3	1.91	0.53
1:B:43:LEU:HD23	1:B:44:THR:N	2.24	0.52
1:C:222:THR:O	1:C:224:THR:HG22	2.10	0.52
1:D:329:LYS:HB2	1:D:333:LEU:CD1	2.39	0.52
1:D:330:THR:OG1	1:D:333:LEU:HG	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:310:GLY:O	1:D:329:LYS:HE2	2.10	0.52
1:D:155:LEU:HD12	1:D:156:VAL:N	2.24	0.52
1:B:54:TRP:CD2	1:B:61:PRO:HB3	2.45	0.52
1:B:70:LEU:N	1:B:85:ASN:HD21	2.02	0.52
1:C:74:GLY:HA3	1:C:76:HIS:CE1	2.45	0.52
1:A:23:TYR:O	1:A:26:VAL:HG22	2.09	0.51
1:C:214:VAL:HB	1:C:215:PRO:HD3	1.92	0.51
1:D:226:VAL:HG22	1:D:320:GLY:O	2.10	0.51
1:B:45:LEU:HD23	1:B:46:GLU:N	2.26	0.51
1:B:54:TRP:CE3	1:B:102:LYS:HE3	2.46	0.51
1:B:66:ILE:HD12	1:B:66:ILE:H	1.75	0.51
1:C:162:SER:O	1:C:163:CYS:HB2	2.10	0.51
1:D:12:LYS:HD3	1:D:357:GLN:NE2	2.27	0.50
1:D:316:SER:HB2	1:D:325:ILE:HG23	1.93	0.50
1:D:341:TRP:HB3	1:D:346:ILE:HB	1.92	0.50
1:D:55:ILE:HD11	1:D:58:TYR:HD2	1.76	0.50
1:A:214:VAL:N	1:A:215:PRO:CD	2.74	0.50
1:B:54:TRP:CZ2	1:B:61:PRO:HG3	2.47	0.50
1:A:20:ALA:HB1	1:A:279:ASN:HD22	1.76	0.50
1:D:173:GLY:HA2	1:D:353:THR:CG2	2.41	0.50
1:B:355:ARG:HG2	1:B:355:ARG:HH11	1.76	0.50
1:A:148:LYS:HB3	1:A:198:MSE:HE1	1.93	0.50
1:C:301:GLU:HB3	1:C:344:LEU:HD13	1.93	0.50
1:C:222:THR:HG21	1:C:299:LEU:HG	1.94	0.50
1:C:228:THR:O	1:C:230:LYS:N	2.45	0.50
1:C:45:LEU:C	1:C:45:LEU:HD23	2.31	0.50
1:C:226:VAL:HG13	1:C:227:SER:N	2.27	0.50
1:B:193:SER:OG	1:B:195:GLU:HG2	2.11	0.50
1:B:226:VAL:O	1:B:227:SER:HB3	2.11	0.50
1:B:239:LYS:HG3	1:B:246:TYR:CD2	2.46	0.50
1:B:88:THR:HG23	1:B:98:LEU:CD1	2.42	0.49
1:A:45:LEU:C	1:A:45:LEU:HD23	2.32	0.49
1:A:173:GLY:HA2	1:A:353:THR:HG21	1.93	0.49
1:A:252:ARG:NH2	1:A:278:GLU:OE1	2.46	0.49
1:D:214:VAL:HB	1:D:215:PRO:HD3	1.95	0.49
1:A:112:GLN:OE1	1:A:112:GLN:N	2.46	0.49
1:D:231:LEU:HA	1:D:234:GLN:OE1	2.13	0.49
1:C:62:VAL:HG13	1:C:77:TRP:CZ2	2.48	0.49
1:D:39:ARG:HH21	1:D:349:LEU:CB	2.23	0.49
1:B:45:LEU:HD23	1:B:45:LEU:C	2.32	0.49
1:B:280:ARG:O	1:B:284:GLN:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:251:THR:O	1:D:255:GLU:HG3	2.13	0.49
1:D:222:THR:HB	1:D:298:LEU:HD23	1.95	0.49
1:D:288:THR:C	1:D:290:ALA:H	2.16	0.49
1:B:43:LEU:HD23	1:B:43:LEU:C	2.34	0.48
1:B:341:TRP:HB3	1:B:346:ILE:HB	1.96	0.48
1:C:239:LYS:HB2	1:C:239:LYS:NZ	2.28	0.48
1:A:88:THR:HG23	1:A:98:LEU:HD11	1.96	0.48
1:D:222:THR:HG21	1:D:299:LEU:HD23	1.96	0.48
1:C:310:GLY:O	1:C:329:LYS:HE2	2.13	0.48
1:B:256:ILE:O	1:B:259:GLN:HB2	2.14	0.48
1:D:74:GLY:HA3	1:D:77:TRP:CD1	2.49	0.48
1:A:194:LEU:H	2:A:1:PGE:C2	2.27	0.48
1:B:39:ARG:NH1	1:B:349:LEU:HD22	2.29	0.48
1:B:226:VAL:HG11	1:B:320:GLY:O	2.14	0.48
1:D:155:LEU:HD12	1:D:155:LEU:C	2.34	0.48
1:D:302:LEU:C	1:D:302:LEU:HD23	2.34	0.48
1:A:274:SER:O	1:A:278:GLU:HG3	2.14	0.47
1:D:300:LYS:HG2	1:D:304:ASP:OD2	2.13	0.47
1:C:215:PRO:HG3	1:C:269:GLU:HG2	1.96	0.47
1:B:230:LYS:HG2	1:B:234:GLN:OE1	2.14	0.47
1:B:251:THR:O	1:B:255:GLU:HG3	2.14	0.47
1:C:228:THR:HG23	1:C:229:GLY:H	1.78	0.47
1:A:277:LYS:NZ	1:A:311:GLY:O	2.47	0.47
1:C:341:TRP:HB3	1:C:346:ILE:HB	1.96	0.47
1:D:43:LEU:C	1:D:43:LEU:HD23	2.35	0.47
1:C:226:VAL:HG22	1:C:228:THR:H	1.79	0.47
1:A:273:TYR:O	1:A:277:LYS:HG3	2.15	0.46
1:C:236:HIS:O	1:C:239:LYS:HG2	2.16	0.46
1:D:45:LEU:C	1:D:45:LEU:HD23	2.36	0.46
1:D:224:THR:O	1:D:225:PRO:C	2.52	0.46
1:B:222:THR:OG1	1:B:298:LEU:HG	2.16	0.46
1:C:309:MSE:HE3	1:C:337:LEU:CA	2.42	0.46
1:D:338:VAL:O	1:D:342:GLU:HG3	2.15	0.46
1:A:66:ILE:HD13	1:A:100:PRO:HD3	1.97	0.46
1:D:16:LYS:HD3	1:D:165:ASP:CB	2.46	0.46
1:B:91:LEU:CD1	1:B:98:LEU:HD21	2.46	0.46
1:B:230:LYS:O	1:B:234:GLN:HG3	2.14	0.46
1:C:38:ASN:ND2	1:C:352:HIS:HB2	2.31	0.46
1:D:331:LYS:NZ	1:D:331:LYS:HB3	2.30	0.46
1:C:292:VAL:HG22	1:C:293:ASN:H	1.80	0.46
1:B:260:ILE:CG1	1:B:275:SER:HB3	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:GLU:HG3	1:C:196:TRP:N	2.31	0.46
1:D:39:ARG:HG2	1:D:39:ARG:HH11	1.81	0.46
1:D:293:ASN:ND2	1:D:296:THR:HG22	2.31	0.46
1:D:332:GLU:HA	1:D:335:GLU:HG3	1.98	0.46
1:B:338:VAL:O	1:B:342:GLU:HG3	2.16	0.45
1:C:280:ARG:O	1:C:284:GLN:HG3	2.15	0.45
1:A:180:PHE:HB3	1:A:205:LEU:HB2	1.98	0.45
1:A:191:TYR:CE1	1:A:192:LYS:HE2	2.51	0.45
1:B:355:ARG:HG2	1:B:355:ARG:NH1	2.31	0.45
1:C:292:VAL:HG22	1:C:293:ASN:N	2.31	0.45
1:B:55:ILE:HD11	1:B:58:TYR:CD2	2.52	0.45
1:A:65:PRO:HG2	1:A:68:GLY:HA3	1.98	0.45
1:D:294:ILE:HG23	1:D:318:SER:O	2.16	0.45
1:B:67:GLY:HA2	1:B:98:LEU:HD12	1.99	0.45
1:D:57:HIS:ND1	1:D:57:HIS:O	2.50	0.45
1:C:180:PHE:HB3	1:C:205:LEU:HB2	1.99	0.45
1:D:12:LYS:HD3	1:D:357:GLN:HE21	1.81	0.45
1:B:334:ALA:O	1:B:338:VAL:HG23	2.16	0.44
1:C:269:GLU:HG3	3:C:443:HOH:O	2.17	0.44
1:D:22:GLU:O	1:D:23:TYR:HB2	2.17	0.44
1:A:20:ALA:HB1	1:A:279:ASN:ND2	2.32	0.44
1:B:260:ILE:HG12	1:B:275:SER:CB	2.48	0.44
1:C:30:HIS:CD2	1:C:254:ASN:ND2	2.84	0.44
1:B:224:THR:O	1:B:224:THR:HG23	2.17	0.44
1:D:217:PHE:CE1	1:D:325:ILE:HB	2.53	0.44
1:B:256:ILE:CD1	1:B:278:GLU:HB3	2.48	0.44
1:D:70:LEU:CD1	1:D:72:PRO:HD3	2.47	0.44
1:A:252:ARG:HG2	1:A:282:ILE:HG21	2.00	0.44
1:C:222:THR:HG21	1:C:299:LEU:CD2	2.47	0.44
1:D:339:ASN:O	1:D:343:LYS:HG3	2.18	0.43
1:D:16:LYS:HD3	1:D:165:ASP:HB3	2.00	0.43
1:B:173:GLY:HA2	1:B:353:THR:HG21	1.99	0.43
1:C:325:ILE:C	1:C:325:ILE:HD12	2.39	0.43
1:C:21:GLY:HA2	1:C:253:ASN:ND2	2.18	0.43
1:D:230:LYS:O	1:D:234:GLN:HG3	2.18	0.43
1:B:296:THR:H	1:B:299:LEU:HD12	1.83	0.43
1:C:189:LEU:HD23	1:C:189:LEU:HA	1.90	0.43
1:C:238:PHE:CE1	1:C:242:ASP:HB3	2.53	0.43
1:B:230:LYS:HB2	1:B:230:LYS:HZ3	1.82	0.43
1:B:339:ASN:O	1:B:343:LYS:HG3	2.18	0.43
1:C:230:LYS:O	1:C:234:GLN:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1:PGE:H6	1:B:194:LEU:HB2	2.00	0.43
1:B:207:ILE:HB	1:C:59:GLU:HB2	2.00	0.43
1:C:22:GLU:O	1:C:23:TYR:HB2	2.18	0.43
1:D:112:GLN:OE1	1:D:112:GLN:N	2.52	0.43
1:C:96:ILE:HG21	1:C:137:PHE:HB3	2.01	0.43
1:D:14:PRO:HB3	1:D:40:TYR:CE1	2.54	0.43
1:D:332:GLU:O	1:D:335:GLU:HB2	2.18	0.43
1:C:31:THR:HG22	1:C:32:ALA:N	2.34	0.43
1:A:21:GLY:N	1:A:279:ASN:HD21	2.12	0.42
1:C:226:VAL:HG22	1:C:228:THR:N	2.33	0.42
1:C:60:ASN:ND2	1:C:61:PRO:HD2	2.33	0.42
1:B:20:ALA:HB1	1:B:279:ASN:ND2	2.33	0.42
1:A:155:LEU:C	1:A:155:LEU:HD12	2.39	0.42
1:B:88:THR:HG23	1:B:98:LEU:HD11	2.02	0.42
1:D:302:LEU:HB2	1:D:346:ILE:HD13	2.01	0.42
1:A:43:LEU:C	1:A:43:LEU:HD23	2.40	0.42
1:A:251:THR:O	1:A:255:GLU:HG3	2.19	0.42
1:A:309:MSE:HE3	1:A:337:LEU:HA	2.02	0.42
1:D:293:ASN:HD21	1:D:296:THR:HG22	1.84	0.42
1:A:112:GLN:CD	1:A:112:GLN:N	2.72	0.42
1:B:22:GLU:CD	1:B:314:LYS:HZ1	2.22	0.42
1:C:138:TYR:CD2	1:C:141:ILE:HB	2.54	0.42
1:D:238:PHE:O	1:D:241:GLU:HB3	2.19	0.42
1:D:341:TRP:O	1:D:344:LEU:N	2.52	0.42
1:B:222:THR:HG23	1:B:299:LEU:HD23	2.01	0.42
1:C:46:GLU:HG2	1:C:102:LYS:HB3	2.01	0.42
1:C:25:VAL:HB	1:C:32:ALA:HB2	2.02	0.42
1:B:41:ILE:HD13	1:B:107:THR:HB	2.02	0.41
1:C:112:GLN:H	1:C:112:GLN:CD	2.23	0.41
1:A:257:MSE:O	1:A:260:ILE:HG22	2.20	0.41
1:C:43:LEU:HD23	1:C:43:LEU:C	2.41	0.41
1:A:293:ASN:ND2	1:A:296:THR:HG22	2.35	0.41
1:C:75:GLU:O	1:C:75:GLU:HG2	2.20	0.41
1:B:43:LEU:HA	1:B:104:VAL:O	2.20	0.41
1:D:257:MSE:HE3	1:D:257:MSE:CA	2.46	0.41
1:B:55:ILE:HG22	1:B:105:ILE:HD12	2.02	0.41
1:B:74:GLY:HA3	1:B:77:TRP:HD1	1.85	0.41
1:B:214:VAL:HB	1:B:269:GLU:OE2	2.21	0.41
1:B:224:THR:O	1:B:225:PRO:C	2.59	0.41
1:D:279:ASN:HD22	1:D:314:LYS:HE3	1.83	0.41
1:D:296:THR:HG23	1:D:320:GLY:HA2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:ILE:HG12	1:B:100:PRO:HD3	2.03	0.41
1:A:90:PHE:CE1	1:A:198:MSE:HG3	2.56	0.40
1:C:351:PHE:CG	1:C:352:HIS:N	2.89	0.40
1:B:196:TRP:CH2	1:B:200:GLU:HG2	2.57	0.40
1:B:231:LEU:N	1:B:231:LEU:HD12	2.36	0.40
1:C:231:LEU:HD11	1:C:320:GLY:HA3	2.04	0.40
1:B:62:VAL:HG13	1:B:77:TRP:CZ2	2.56	0.40
1:B:66:ILE:HD12	1:B:66:ILE:N	2.37	0.40
1:B:183:GLU:HG3	3:B:373:HOH:O	2.21	0.40
1:C:155:LEU:C	1:C:155:LEU:CD1	2.90	0.40
1:D:349:LEU:O	1:D:350:PRO:C	2.60	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	353/365 (97%)	342 (97%)	11 (3%)	0	100	100
1	B	353/365 (97%)	335 (95%)	16 (4%)	2 (1%)	25	21
1	C	353/365 (97%)	336 (95%)	11 (3%)	6 (2%)	9	4
1	D	353/365 (97%)	322 (91%)	24 (7%)	7 (2%)	7	3
All	All	1412/1460 (97%)	1335 (94%)	62 (4%)	15 (1%)	14	9

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	227	SER
1	C	223	GLY
1	C	226	VAL
1	C	228	THR

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Mol	Chain	Res	Type
1	C	229	GLY
1	D	223	GLY
1	B	112	GLN
1	C	227	SER
1	D	225	PRO
1	D	289	LYS
1	D	74	GLY
1	D	241	GLU
1	D	288	THR
1	C	56	PRO
1	D	350	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	298/299 (100%)	295 (99%)	3 (1%)	76	82
1	B	298/299 (100%)	293 (98%)	5 (2%)	60	67
1	C	298/299 (100%)	292 (98%)	6 (2%)	55	60
1	D	298/299 (100%)	291 (98%)	7 (2%)	50	55
All	All	1192/1196 (100%)	1171 (98%)	21 (2%)	59	65

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	112	GLN
1	A	155	LEU
1	B	16	LYS
1	B	39	ARG
1	B	54	TRP
1	B	222	THR
1	B	309	MSE
1	C	16	LYS
1	C	56	PRO

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Mol	Chain	Res	Type
1	C	155	LEU
1	C	195	GLU
1	C	199	LYS
1	C	239	LYS
1	D	16	LYS
1	D	138	TYR
1	D	188	ARG
1	D	225	PRO
1	D	257	MSE
1	D	339	ASN
1	D	340	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	240	GLN
1	A	245	ASN
1	A	247	GLN
1	A	253	ASN
1	A	279	ASN
1	A	348	HIS
1	A	352	HIS
1	B	60	ASN
1	B	85	ASN
1	B	131	ASN
1	B	240	GLN
1	B	245	ASN
1	B	253	ASN
1	B	259	GLN
1	B	279	ASN
1	B	293	ASN
1	C	60	ASN
1	C	85	ASN
1	C	182	GLN
1	C	253	ASN
1	C	254	ASN
1	C	279	ASN
1	C	339	ASN
1	C	348	HIS
1	D	85	ASN
1	D	131	ASN

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Mol	Chain	Res	Type
1	D	240	GLN
1	D	245	ASN
1	D	253	ASN
1	D	279	ASN
1	D	293	ASN
1	D	339	ASN
1	D	357	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	PGE	A	1	-	9,9,9	0.93	0	8,8,8	2.57	3 (37%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PGE	A	1	-	-	3/7/7/7	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	PGE	O3-C4-C3	-5.00	87.57	110.35
2	A	1	PGE	C3-O2-C2	-4.28	94.52	113.26
2	A	1	PGE	O3-C5-C6	-2.14	100.67	110.11

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	PGE	O2-C3-C4-O3
2	A	1	PGE	O1-C1-C2-O2
2	A	1	PGE	O3-C5-C6-O4

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	PGE	4	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	347/365 (95%)	0.17	5 (1%) 75 78	12, 24, 45, 65	0
1	B	347/365 (95%)	0.52	21 (6%) 21 26	16, 37, 63, 81	0
1	C	347/365 (95%)	0.24	10 (2%) 51 57	13, 24, 51, 75	0
1	D	347/365 (95%)	1.02	59 (17%) 1 1	17, 40, 73, 90	0
All	All	1388/1460 (95%)	0.49	95 (6%) 17 21	12, 30, 66, 90	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	223	GLY	18.9
1	D	229	GLY	17.4
1	D	226	VAL	14.8
1	C	224	THR	11.2
1	B	361	GLY	8.9
1	D	228	THR	8.8
1	C	226	VAL	8.0
1	C	227	SER	7.2
1	C	228	THR	5.9
1	C	229	GLY	5.4
1	B	227	SER	5.2
1	B	222	THR	5.2
1	D	223	GLY	5.1
1	D	345	GLY	4.7
1	B	7	ASN	4.6
1	B	225	PRO	4.5
1	D	339	ASN	4.5
1	D	291	GLY	4.4
1	D	245	ASN	4.4
1	D	112	GLN	4.0
1	B	228	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	224	THR	3.8
1	D	113	SER	3.8
1	B	54	TRP	3.8
1	D	352	HIS	3.7
1	D	293	ASN	3.7
1	B	229	GLY	3.6
1	B	360	GLU	3.5
1	B	112	GLN	3.5
1	B	226	VAL	3.5
1	D	332	GLU	3.4
1	D	294	ILE	3.4
1	D	225	PRO	3.4
1	D	155	LEU	3.3
1	D	117	TYR	3.3
1	D	110	ILE	3.3
1	D	114	GLY	3.3
1	D	289	LYS	3.1
1	D	301	GLU	3.1
1	B	9	LEU	3.1
1	D	73	ASP	3.0
1	B	293	ASN	3.0
1	D	320	GLY	2.9
1	D	244	LYS	2.9
1	C	351	PHE	2.9
1	D	57	HIS	2.9
1	D	59	GLU	2.9
1	D	349	LEU	2.9
1	B	224	THR	2.8
1	D	359	THR	2.8
1	D	338	VAL	2.7
1	B	339	ASN	2.7
1	D	343	LYS	2.7
1	D	238	PHE	2.7
1	D	288	THR	2.7
1	D	340	GLU	2.7
1	D	221	TRP	2.7
1	D	231	LEU	2.7
1	D	344	LEU	2.7
1	C	138	TYR	2.7
1	D	49	GLU	2.6
1	D	54	TRP	2.6
1	D	227	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	237	ALA	2.6
1	D	306	ALA	2.5
1	D	111	ASP	2.5
1	D	230	LYS	2.5
1	D	232	VAL	2.4
1	A	361	GLY	2.4
1	D	281	ARG	2.4
1	D	308	ASN	2.4
1	A	244	LYS	2.4
1	A	241	GLU	2.4
1	D	58	TYR	2.4
1	B	49	GLU	2.4
1	D	335	GLU	2.3
1	D	346	ILE	2.3
1	D	252	ARG	2.2
1	D	235	ILE	2.2
1	D	292	VAL	2.2
1	B	342	GLU	2.2
1	D	331	LYS	2.2
1	C	230	LYS	2.2
1	B	336	LYS	2.1
1	C	225	PRO	2.1
1	A	7	ASN	2.1
1	B	57	HIS	2.1
1	D	115	ALA	2.1
1	B	231	LEU	2.0
1	A	227	SER	2.0
1	D	243	SER	2.0
1	B	223	GLY	2.0
1	D	242	ASP	2.0
1	D	341	TRP	2.0
1	D	250	LEU	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 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<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(Å <sup>2</sup> )	Q<0.9
2	PGE	A	1	10/10	0.60	0.33	35,46,49,50	0

## 6.5 Other polymers

There are no such residues in this entry.