



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:18 AM GMT

PDB ID : 2GGH
Title : The mutant A68C-D72C-NLQ of Deinococcus Radiodurans Nacylamino acid racemase
Authors : Wang, W.C.; Chiu, W.C.
Deposited on : 2006-03-24
Resolution : 2.20 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

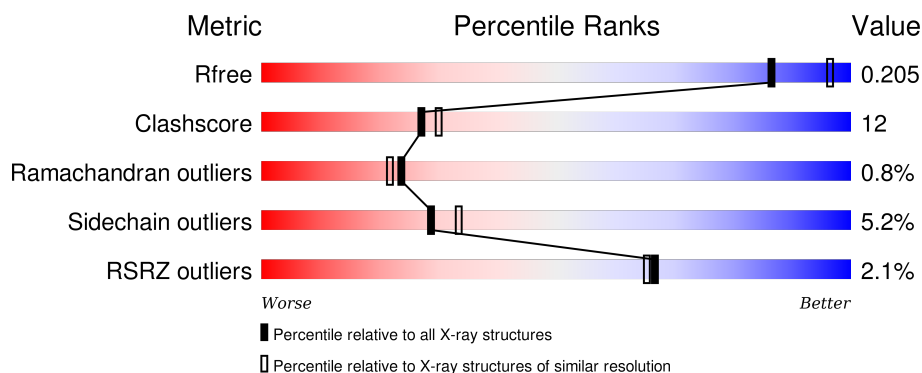
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION





The reported resolution of this entry is 2.20 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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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. 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	375	 83% 11% . .
1	B	375	 86% 10% . .
1	C	375	 5% 73% 21% . .
1	D	375	 4% 79% 15% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	A	1377	-	-	-	X
2	MG	B	2377	-	-	-	X
3	NLQ	C	1376	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11964 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 N-acylamino acid racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	0	0	0
			2765	1732	507	514	12			
1	B	360	Total	C	N	O	S	0	0	0
			2765	1732	507	514	12			
1	C	370	Total	C	N	O	S	0	0	0
			2851	1789	521	529	12			
1	D	370	Total	C	N	O	S	0	0	0
			2851	1789	521	529	12			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	CYS	ALA	ENGINEERED	UNP Q9RYA6
A	72	CYS	ASP	ENGINEERED	UNP Q9RYA6
A	94	SER	ALA	SEE REMARK 999	UNP Q9RYA6
A	148	ASP	GLY	SEE REMARK 999	UNP Q9RYA6
A	158	ARG	LYS	SEE REMARK 999	UNP Q9RYA6
A	252	SER	ALA	SEE REMARK 999	UNP Q9RYA6
A	315	SER	PRO	SEE REMARK 999	UNP Q9RYA6
B	68	CYS	ALA	ENGINEERED	UNP Q9RYA6
B	72	CYS	ASP	ENGINEERED	UNP Q9RYA6
B	94	SER	ALA	SEE REMARK 999	UNP Q9RYA6
B	148	ASP	GLY	SEE REMARK 999	UNP Q9RYA6
B	158	ARG	LYS	SEE REMARK 999	UNP Q9RYA6
B	252	SER	ALA	SEE REMARK 999	UNP Q9RYA6
B	315	SER	PRO	SEE REMARK 999	UNP Q9RYA6
C	68	CYS	ALA	ENGINEERED	UNP Q9RYA6
C	72	CYS	ASP	ENGINEERED	UNP Q9RYA6
C	94	SER	ALA	SEE REMARK 999	UNP Q9RYA6
C	148	ASP	GLY	SEE REMARK 999	UNP Q9RYA6
C	158	ARG	LYS	SEE REMARK 999	UNP Q9RYA6
C	252	SER	ALA	SEE REMARK 999	UNP Q9RYA6
C	315	SER	PRO	SEE REMARK 999	UNP Q9RYA6

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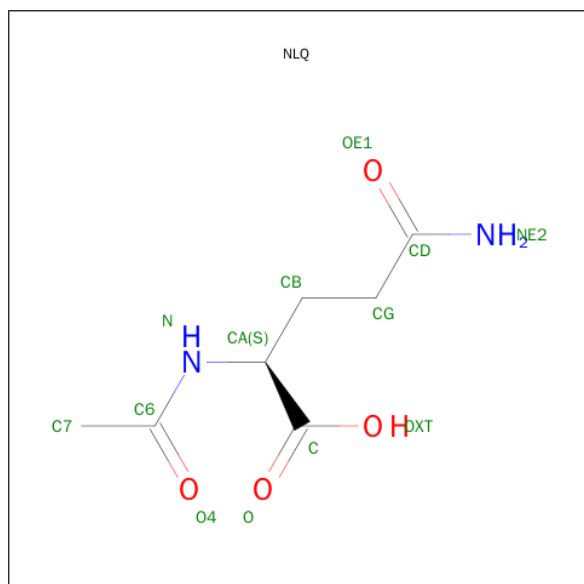
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Chain	Residue	Modelled	Actual	Comment	Reference
D	68	CYS	ALA	ENGINEERED	UNP Q9RYA6
D	72	CYS	ASP	ENGINEERED	UNP Q9RYA6
D	94	SER	ALA	SEE REMARK 999	UNP Q9RYA6
D	148	ASP	GLY	SEE REMARK 999	UNP Q9RYA6
D	158	ARG	LYS	SEE REMARK 999	UNP Q9RYA6
D	252	SER	ALA	SEE REMARK 999	UNP Q9RYA6
D	315	SER	PRO	SEE REMARK 999	UNP Q9RYA6

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

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

- Molecule 3 is N²-ACETYL-L-GLUTAMINE (three-letter code: NLQ) (formula: C₇H₁₂N₂O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C N O 13 7 2 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	0	0
			13	7	2	4		

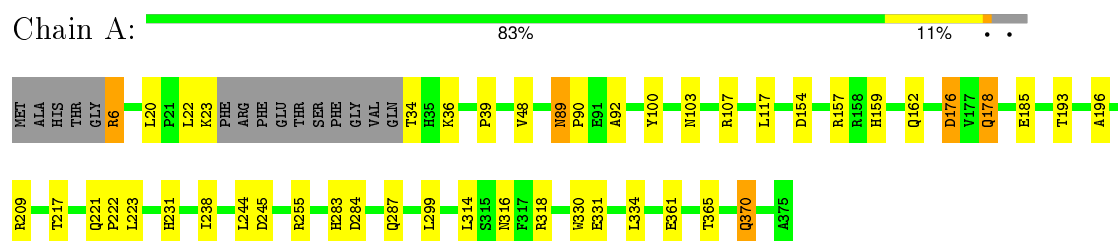
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	200	Total	O	0	0
			200	200		
4	B	198	Total	O	0	0
			198	198		
4	C	153	Total	O	0	0
			153	153		
4	D	151	Total	O	0	0
			151	151		

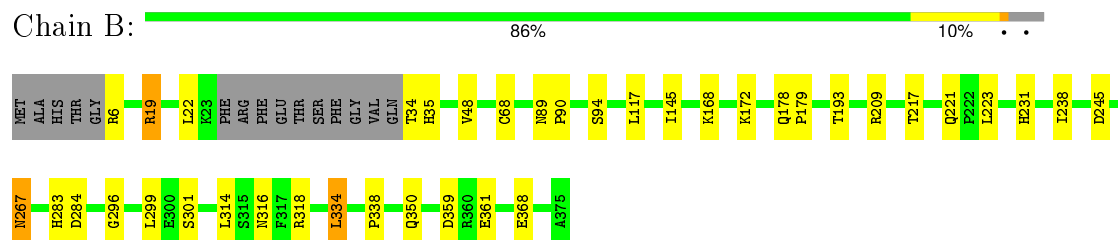
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

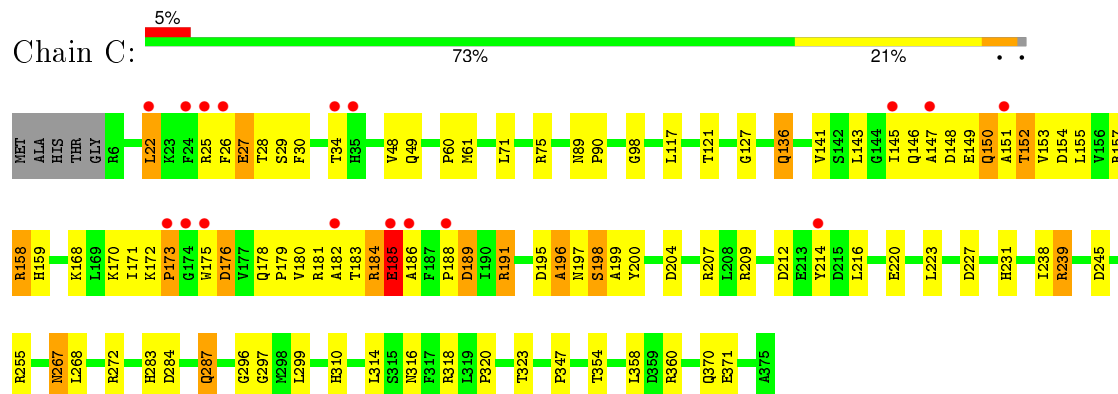
• Molecule 1: N-acylamino acid racemase



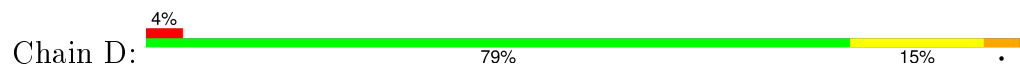
• Molecule 1: N-acylamino acid racemase

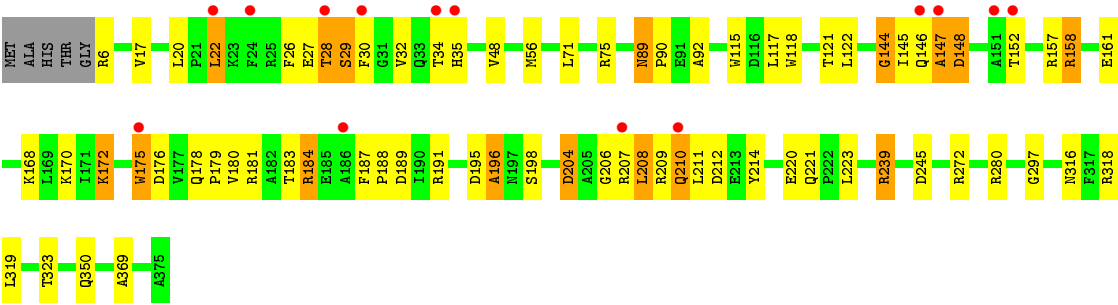


• Molecule 1: N-acylamino acid racemase



• Molecule 1: N-acylamino acid racemase





4 Data and refinement statistics

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α , β , γ	116.19Å 116.19Å 120.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 29.05 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.7 (30.00-2.20) 98.7 (29.05-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.43 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.188 , 0.228 0.190 , 0.205	Depositor DCC
R_{free} test set	4030 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 14.0	EDS
Estimated twinning fraction	0.000 for -h,-l,-k 0.000 for -h,l,k 0.002 for l,-k,h 0.005 for -l,-k,-h 0.487 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 80201 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11964	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: NLQ, MG

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	0.49	0/2816	0.62	0/3820
1	B	0.49	0/2816	0.61	0/3820
1	C	0.46	0/2906	0.60	0/3942
1	D	0.46	0/2906	0.61	0/3942
All	All	0.48	0/11444	0.61	0/15524

There are no bond length outliers.

There are no bond angle outliers.

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	2765	0	2768	45	0
1	B	2765	0	2768	31	0
1	C	2851	0	2847	118	0
1	D	2851	0	2847	78	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	C	13	0	11	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	13	0	11	2	0
4	A	200	0	0	6	0
4	B	198	0	0	3	0
4	C	153	0	0	7	0
4	D	151	0	0	5	0
All	All	11964	0	11252	270	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 12.

All (270) 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:184:ARG:HG2	1:C:184:ARG:HH21	1.12	1.13
1:D:239:ARG:HG2	1:D:239:ARG:HH21	1.09	1.08
1:C:27:GLU:O	1:C:27:GLU:HG3	1.31	1.07
1:D:158:ARG:HB2	1:D:158:ARG:NH1	1.72	1.03
1:A:154:ASP:HB2	4:A:1518:HOH:O	1.60	1.02
1:D:297:GLY:O	3:D:2376:NLQ:HB2	1.59	1.01
1:C:184:ARG:HH21	1:C:184:ARG:CG	1.74	0.99
1:C:178:GLN:HB2	1:C:179:PRO:HD3	1.43	0.97
1:D:27:GLU:H	1:D:32:VAL:HA	1.29	0.97
1:C:22:LEU:HB2	1:C:34:THR:O	1.65	0.96
1:C:158:ARG:HH21	1:C:158:ARG:HG3	1.27	0.96
1:D:158:ARG:HB2	1:D:158:ARG:HH11	1.30	0.93
1:D:27:GLU:HG3	1:D:145:ILE:HB	1.51	0.92
1:D:22:LEU:HB2	1:D:34:THR:O	1.69	0.92
1:A:178:GLN:H	1:A:178:GLN:HE21	0.96	0.92
1:C:28:THR:HG22	1:C:30:PHE:H	1.35	0.91
1:C:158:ARG:HH21	1:C:158:ARG:CG	1.85	0.90
1:C:27:GLU:O	1:C:27:GLU:CG	2.19	0.90
1:C:184:ARG:NH2	1:C:184:ARG:HG2	1.80	0.89
1:D:239:ARG:NH2	1:D:239:ARG:HG2	1.88	0.87
1:C:297:GLY:O	3:C:1376:NLQ:HB3	1.75	0.86
1:A:221:GLN:NE2	1:A:245:ASP:H	1.72	0.86
1:B:221:GLN:NE2	1:B:245:ASP:H	1.74	0.85
1:A:316:ASN:HD22	1:A:318:ARG:HE	1.23	0.84
1:D:172:LYS:NZ	1:D:175:TRP:HB2	1.93	0.83
1:C:181:ARG:HG2	1:C:181:ARG:HH11	1.40	0.83
1:A:287:GLN:HE22	1:A:318:ARG:HH21	1.27	0.83
1:D:210:GLN:OE1	1:D:210:GLN:HA	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:GLN:HE21	1:C:155:LEU:HD22	1.45	0.81
1:A:178:GLN:H	1:A:178:GLN:NE2	1.78	0.80
1:A:36:LYS:HD2	1:A:299:LEU:HD23	1.64	0.80
1:D:145:ILE:HG23	4:D:4423:HOH:O	1.82	0.79
1:B:316:ASN:HD22	1:B:318:ARG:HE	1.31	0.79
1:A:221:GLN:HE21	1:A:245:ASP:H	1.30	0.78
1:D:316:ASN:HD22	1:D:318:ARG:HE	1.28	0.78
1:A:107:ARG:HD2	4:A:1489:HOH:O	1.82	0.77
1:C:136:GLN:HB3	1:C:347:PRO:HA	1.67	0.77
1:A:48:VAL:HG23	1:A:117:LEU:HD12	1.67	0.77
1:C:158:ARG:NH2	1:C:158:ARG:HG3	2.00	0.77
1:A:283:HIS:HE1	1:A:316:ASN:H	1.31	0.76
1:B:48:VAL:HG23	1:B:117:LEU:HD12	1.67	0.76
1:D:239:ARG:CG	1:D:239:ARG:HH21	1.93	0.76
1:D:184:ARG:O	1:D:188:PRO:HA	1.86	0.76
1:B:267:ASN:HD21	1:B:296:GLY:HA3	1.48	0.76
1:C:28:THR:HG23	1:C:197:ASN:HD21	1.51	0.74
1:B:283:HIS:HE1	1:B:316:ASN:H	1.35	0.74
1:C:283:HIS:CE1	1:C:316:ASN:H	2.05	0.74
1:C:181:ARG:HB2	1:C:214:TYR:CZ	2.22	0.74
1:D:27:GLU:HB3	4:D:4464:HOH:O	1.85	0.74
1:A:178:GLN:N	1:A:178:GLN:HE21	1.80	0.73
1:D:28:THR:O	1:D:29:SER:HB3	1.87	0.73
1:A:283:HIS:CE1	1:A:316:ASN:H	2.06	0.73
1:C:283:HIS:HE1	1:C:316:ASN:H	1.34	0.73
1:D:178:GLN:HG3	1:D:181:ARG:HH12	1.55	0.72
1:B:283:HIS:CE1	1:B:316:ASN:H	2.07	0.72
1:D:172:LYS:HZ2	1:D:175:TRP:HB2	1.53	0.71
1:D:172:LYS:HZ2	1:D:175:TRP:CB	2.03	0.71
1:C:173:PRO:CD	1:C:199:ALA:HB1	2.20	0.71
1:D:198:SER:HB2	1:D:223:LEU:O	1.90	0.71
1:C:168:LYS:HE3	1:C:195:ASP:HB2	1.73	0.70
1:C:170:LYS:HE2	1:C:195:ASP:OD2	1.91	0.70
1:C:170:LYS:HD2	1:C:197:ASN:ND2	2.07	0.70
1:C:178:GLN:HB2	1:C:179:PRO:CD	2.20	0.69
1:B:267:ASN:C	1:B:267:ASN:HD22	1.95	0.69
1:B:19:ARG:HG3	1:B:368:GLU:OE1	1.94	0.68
1:D:28:THR:O	1:D:29:SER:CB	2.42	0.67
1:C:27:GLU:CG	1:C:145:ILE:HB	2.23	0.67
1:D:184:ARG:O	1:D:184:ARG:HG3	1.95	0.67
1:C:27:GLU:HG2	1:C:145:ILE:HB	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:HIS:HD2	1:C:284:ASP:OD1	1.79	0.66
1:C:267:ASN:HD21	1:C:296:GLY:HA3	1.60	0.65
1:B:316:ASN:ND2	1:B:318:ARG:HE	1.94	0.65
1:D:28:THR:HG21	1:D:30:PHE:CE1	2.32	0.65
1:A:22:LEU:HD12	1:A:34:THR:HG23	1.77	0.65
1:C:181:ARG:HH11	1:C:181:ARG:CG	2.09	0.65
1:C:209:ARG:HD2	4:C:3506:HOH:O	1.96	0.64
1:B:221:GLN:HE21	1:B:245:ASP:H	1.44	0.64
1:C:71:LEU:O	1:C:75:ARG:HG2	1.96	0.64
1:C:197:ASN:O	1:C:199:ALA:N	2.30	0.64
1:D:145:ILE:HA	1:D:146:GLN:OE1	1.96	0.64
1:C:287:GLN:HE22	1:C:318:ARG:HH11	1.46	0.63
1:C:267:ASN:HD22	1:C:267:ASN:C	2.02	0.63
1:B:6:ARG:N	4:B:2503:HOH:O	2.30	0.63
1:C:29:SER:H	1:C:197:ASN:ND2	1.96	0.62
1:D:22:LEU:CB	1:D:34:THR:O	2.44	0.62
1:B:283:HIS:HD2	1:B:284:ASP:OD1	1.82	0.62
1:B:316:ASN:HD22	1:B:318:ARG:NE	1.97	0.62
1:D:195:ASP:O	1:D:196:ALA:HB2	2.00	0.62
1:C:117:LEU:O	1:C:121:THR:HG23	2.00	0.62
1:C:297:GLY:O	3:C:1376:NLQ:CB	2.46	0.61
1:C:28:THR:CG2	1:C:29:SER:N	2.64	0.61
1:D:175:TRP:HA	1:D:175:TRP:CE3	2.36	0.61
1:A:20:LEU:HD13	1:A:334:LEU:HD21	1.83	0.61
1:D:71:LEU:O	1:D:75:ARG:HG2	2.00	0.61
1:A:6:ARG:N	4:A:1503:HOH:O	2.33	0.61
1:C:26:PHE:CE2	3:C:1376:NLQ:HA	2.36	0.60
1:A:283:HIS:HD2	1:A:284:ASP:OD1	1.84	0.60
1:A:103:ASN:O	1:A:107:ARG:HG3	2.02	0.60
1:D:206:GLY:C	1:D:208:LEU:H	2.06	0.60
1:A:287:GLN:HE22	1:A:318:ARG:NH2	2.00	0.59
1:D:157:ARG:O	1:D:161:GLU:HG3	2.03	0.59
1:D:89:ASN:ND2	1:D:92:ALA:H	2.00	0.59
1:C:153:VAL:HG21	1:C:182:ALA:O	2.03	0.58
1:A:316:ASN:ND2	1:A:318:ARG:HE	1.97	0.58
1:B:301:SER:OG	1:B:334:LEU:HD11	2.03	0.58
1:B:283:HIS:CE1	1:B:314:LEU:HB3	2.39	0.57
1:C:48:VAL:HG23	1:C:117:LEU:HD12	1.85	0.57
1:D:175:TRP:HA	1:D:175:TRP:HE3	1.70	0.56
1:D:27:GLU:CG	1:D:145:ILE:HB	2.28	0.56
1:D:175:TRP:CE2	1:D:179:PRO:HG3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:SER:HB3	1:D:221:GLN:HG3	1.88	0.56
1:C:127:GLY:H	1:C:310:HIS:CD2	2.24	0.56
1:C:29:SER:H	1:C:197:ASN:HD21	1.51	0.56
1:C:223:LEU:H	1:C:231:HIS:CE1	2.22	0.56
1:C:209:ARG:O	1:C:212:ASP:HB2	2.06	0.56
1:D:350:GLN:HG2	4:D:4471:HOH:O	2.04	0.56
1:C:179:PRO:O	1:C:183:THR:N	2.39	0.56
1:C:158:ARG:HH21	1:C:158:ARG:CB	2.18	0.56
1:C:283:HIS:CE1	1:C:314:LEU:HB3	2.41	0.55
1:B:223:LEU:H	1:B:231:HIS:CE1	2.23	0.55
1:C:173:PRO:HD3	1:C:199:ALA:CB	2.36	0.55
1:C:184:ARG:NH2	1:C:184:ARG:CG	2.45	0.55
1:D:316:ASN:ND2	1:D:318:ARG:HE	2.02	0.55
1:C:209:ARG:HB2	1:C:238:ILE:HG22	1.88	0.55
1:D:183:THR:O	1:D:187:PHE:N	2.36	0.55
1:A:48:VAL:HG23	1:A:117:LEU:CD1	2.37	0.55
1:C:227:ASP:OD2	1:C:231:HIS:HD2	1.89	0.55
1:C:153:VAL:CG2	1:C:182:ALA:O	2.54	0.54
1:A:223:LEU:H	1:A:231:HIS:CE1	2.25	0.54
1:B:94:SER:HB2	4:B:2529:HOH:O	2.06	0.54
1:A:370:GLN:HG2	4:A:1514:HOH:O	2.07	0.54
1:D:89:ASN:HD22	1:D:92:ALA:H	1.55	0.54
1:C:150:GLN:HB3	4:C:3481:HOH:O	2.07	0.54
1:B:48:VAL:HG23	1:B:117:LEU:CD1	2.38	0.54
1:A:283:HIS:CE1	1:A:314:LEU:HB3	2.42	0.54
1:D:198:SER:CB	1:D:223:LEU:O	2.54	0.54
1:D:144:GLY:O	1:D:146:GLN:OE1	2.27	0.53
1:C:158:ARG:NH2	1:C:158:ARG:CG	2.56	0.53
1:D:204:ASP:N	1:D:204:ASP:OD1	2.41	0.53
1:A:159:HIS:HD2	1:A:162:GLN:OE1	1.90	0.53
1:C:49:GLN:HE22	1:C:360:ARG:HH22	1.56	0.53
1:C:182:ALA:HA	1:C:185:GLU:HB2	1.90	0.53
1:C:22:LEU:CB	1:C:34:THR:O	2.49	0.53
4:A:1486:HOH:O	1:C:198:SER:HB2	2.09	0.53
1:D:316:ASN:HD22	1:D:318:ARG:NE	2.02	0.53
1:C:61:MET:HE1	4:C:3508:HOH:O	2.09	0.53
1:C:29:SER:OG	1:C:197:ASN:CG	2.47	0.53
1:D:117:LEU:O	1:D:121:THR:HG23	2.09	0.53
1:C:145:ILE:HG23	4:C:3480:HOH:O	2.08	0.52
1:A:36:LYS:NZ	4:A:1542:HOH:O	2.42	0.52
1:D:175:TRP:HD1	4:D:4423:HOH:O	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:ASP:HB2	4:C:3463:HOH:O	2.10	0.52
1:C:195:ASP:HA	1:C:220:GLU:HB3	1.92	0.52
1:C:127:GLY:H	1:C:310:HIS:HD2	1.57	0.52
1:D:297:GLY:HA3	3:D:2376:NLQ:HE21	1.74	0.52
1:C:180:VAL:O	1:C:184:ARG:HB2	2.10	0.52
1:D:195:ASP:O	1:D:196:ALA:CB	2.58	0.52
1:D:35:HIS:HB2	4:D:4440:HOH:O	2.10	0.52
1:D:158:ARG:HB2	1:D:158:ARG:CZ	2.37	0.51
1:C:28:THR:HG21	1:C:30:PHE:CE2	2.45	0.51
1:C:267:ASN:HD21	1:C:296:GLY:CA	2.21	0.51
1:C:26:PHE:HE2	3:C:1376:NLQ:HA	1.74	0.51
1:C:29:SER:OG	1:C:197:ASN:OD1	2.27	0.51
1:C:245:ASP:OD1	1:C:272:ARG:NH2	2.44	0.50
1:A:89:ASN:ND2	1:A:92:ALA:H	2.08	0.50
1:C:310:HIS:HE1	1:C:354:THR:O	1.94	0.50
1:C:158:ARG:HH21	1:C:158:ARG:HB2	1.77	0.50
1:C:154:ASP:O	1:C:157:ARG:HB3	2.12	0.50
1:A:89:ASN:HD22	1:A:92:ALA:H	1.60	0.50
1:C:171:ILE:CG1	1:C:196:ALA:HA	2.42	0.50
1:D:147:ALA:O	1:D:148:ASP:HB3	2.11	0.49
1:D:144:GLY:HA2	1:D:170:LYS:HG3	1.94	0.49
1:A:222:PRO:HD2	1:A:231:HIS:CE1	2.46	0.49
1:C:48:VAL:HG23	1:C:117:LEU:CD1	2.42	0.49
1:C:180:VAL:HG13	1:C:216:LEU:HD21	1.93	0.49
1:C:173:PRO:HD3	1:C:199:ALA:HB1	1.93	0.48
1:C:28:THR:HG23	1:C:29:SER:H	1.78	0.48
1:B:209:ARG:HB2	1:B:238:ILE:HG22	1.95	0.48
1:D:28:THR:HG21	1:D:30:PHE:CZ	2.47	0.48
1:B:361:GLU:H	1:B:361:GLU:CD	2.17	0.48
1:C:171:ILE:HB	1:C:176:ASP:HB3	1.96	0.48
1:C:27:GLU:HG3	1:C:145:ILE:HB	1.95	0.48
1:A:222:PRO:HD2	1:A:231:HIS:HE1	1.79	0.48
1:A:287:GLN:NE2	1:A:318:ARG:HH21	2.06	0.47
1:C:143:LEU:HD21	1:C:159:HIS:CE1	2.49	0.47
1:B:145:ILE:HD13	1:B:172:LYS:HD3	1.97	0.47
1:D:195:ASP:HA	1:D:220:GLU:HB3	1.97	0.47
1:C:153:VAL:HG12	1:C:153:VAL:O	2.15	0.47
1:C:186:ALA:C	1:C:188:PRO:HD3	2.35	0.46
1:C:28:THR:HG23	1:C:29:SER:N	2.30	0.46
1:D:191:ARG:HH12	1:D:319:LEU:CD2	2.28	0.46
1:C:75:ARG:HD2	4:C:3451:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:195:ASP:CG	1:D:196:ALA:H	2.19	0.46
1:D:27:GLU:N	1:D:32:VAL:HA	2.12	0.46
1:C:28:THR:HB	4:C:3450:HOH:O	2.15	0.46
1:A:157:ARG:HG2	1:B:338:PRO:HG3	1.98	0.46
1:C:181:ARG:HB2	1:C:214:TYR:CE2	2.50	0.46
1:C:150:GLN:C	1:C:152:THR:H	2.18	0.46
1:B:267:ASN:C	1:B:267:ASN:ND2	2.65	0.45
1:A:89:ASN:HB2	1:A:90:PRO:CD	2.47	0.45
1:D:28:THR:HG21	1:D:30:PHE:CD1	2.52	0.45
1:D:148:ASP:C	1:D:148:ASP:OD1	2.55	0.45
1:C:195:ASP:O	1:C:197:ASN:N	2.50	0.45
1:B:34:THR:OG1	1:B:35:HIS:HD2	1.99	0.45
1:D:157:ARG:HA	1:D:187:PHE:CZ	2.51	0.45
1:C:267:ASN:ND2	1:C:267:ASN:C	2.68	0.45
1:C:180:VAL:HG12	1:C:214:TYR:CB	2.46	0.45
1:D:28:THR:HG22	1:D:30:PHE:H	1.82	0.45
1:D:204:ASP:O	1:D:208:LEU:HB2	2.16	0.45
1:C:89:ASN:HB2	1:C:90:PRO:CD	2.47	0.45
1:A:100:TYR:HB3	1:C:60:PRO:HG2	2.00	0.44
1:D:206:GLY:C	1:D:208:LEU:N	2.71	0.44
1:D:158:ARG:CB	1:D:158:ARG:HH11	2.17	0.44
1:C:29:SER:HG	1:C:197:ASN:CG	2.18	0.44
1:D:178:GLN:N	1:D:179:PRO:HD2	2.33	0.44
1:D:198:SER:HB3	1:D:221:GLN:CG	2.47	0.44
1:D:209:ARG:O	1:D:212:ASP:HB2	2.17	0.44
1:B:178:GLN:N	1:B:179:PRO:HD2	2.32	0.44
1:D:48:VAL:HG23	1:D:117:LEU:HD12	2.00	0.44
1:C:227:ASP:OD2	1:C:231:HIS:CD2	2.68	0.44
1:C:148:ASP:C	1:C:148:ASP:OD1	2.57	0.44
1:D:245:ASP:OD2	1:D:272:ARG:NH2	2.50	0.44
1:D:146:GLN:HB3	1:D:147:ALA:H	1.67	0.44
1:D:172:LYS:O	1:D:172:LYS:HD2	2.18	0.43
1:C:89:ASN:HB2	1:C:90:PRO:HD2	1.98	0.43
1:C:200:TYR:HB3	1:C:204:ASP:HB2	2.00	0.43
1:A:176:ASP:H	1:A:178:GLN:HE22	1.65	0.43
1:C:170:LYS:CD	1:C:197:ASN:ND2	2.79	0.43
1:C:28:THR:HG21	1:C:30:PHE:CD2	2.53	0.43
1:C:186:ALA:O	1:C:188:PRO:HD3	2.17	0.43
1:C:299:LEU:HD23	3:C:1376:NLQ:HG2	2.00	0.43
1:D:168:LYS:HE3	1:D:195:ASP:HB2	2.00	0.43
1:A:255:ARG:HD2	1:A:255:ARG:C	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:PRO:CD	1:C:199:ALA:CB	2.89	0.43
1:D:89:ASN:HD22	1:D:89:ASN:C	2.21	0.43
1:A:209:ARG:HB2	1:A:238:ILE:HG22	2.00	0.43
1:C:212:ASP:OD1	1:C:239:ARG:HB2	2.19	0.42
1:B:359:ASP:OD2	1:B:361:GLU:HG2	2.19	0.42
1:D:90:PRO:HG2	1:D:115:TRP:CD2	2.54	0.42
1:C:191:ARG:HH21	1:C:320:PRO:HD3	1.84	0.42
1:C:178:GLN:CB	1:C:179:PRO:HD3	2.30	0.42
1:A:316:ASN:HD22	1:A:318:ARG:NE	2.04	0.42
1:B:19:ARG:HD3	1:B:35:HIS:HB3	2.02	0.42
1:C:267:ASN:HD22	1:C:268:LEU:N	2.18	0.42
1:D:323:THR:HG22	1:D:323:THR:O	2.20	0.42
1:C:148:ASP:OD1	1:C:151:ALA:N	2.46	0.42
1:D:180:VAL:HG12	1:D:214:TYR:CD2	2.55	0.41
1:A:193:THR:HG22	1:A:217:THR:HB	2.02	0.41
1:A:22:LEU:HD23	1:A:330:TRP:CZ3	2.55	0.41
1:C:358:LEU:HD23	1:C:358:LEU:HA	1.88	0.41
1:B:193:THR:HG22	1:B:217:THR:HB	2.02	0.41
1:C:197:ASN:C	1:C:199:ALA:N	2.74	0.41
1:C:197:ASN:O	1:C:198:SER:C	2.58	0.41
1:A:196:ALA:HB3	1:A:222:PRO:HA	2.02	0.41
1:D:239:ARG:NH2	1:D:239:ARG:CG	2.63	0.41
1:A:89:ASN:HB2	1:A:90:PRO:HD2	2.01	0.41
1:D:17:VAL:HB	1:D:369:ALA:HB3	2.01	0.41
1:A:176:ASP:H	1:A:178:GLN:NE2	2.19	0.41
1:B:221:GLN:HE21	1:B:245:ASP:N	2.16	0.41
1:B:89:ASN:HB2	1:B:90:PRO:CD	2.51	0.41
1:A:361:GLU:O	1:A:365:THR:HG23	2.21	0.41
1:C:310:HIS:CE1	1:C:354:THR:O	2.73	0.40
1:C:148:ASP:OD1	1:C:151:ALA:HB3	2.21	0.40
1:D:118:TRP:CZ2	1:D:122:LEU:HD11	2.56	0.40
1:C:323:THR:O	1:C:323:THR:HG22	2.21	0.40
1:C:283:HIS:CE1	1:C:316:ASN:HB3	2.56	0.40
1:A:89:ASN:HD22	1:A:89:ASN:C	2.25	0.40
1:C:255:ARG:HD2	1:C:255:ARG:C	2.41	0.40
1:B:94:SER:CB	4:B:2529:HOH:O	2.68	0.40
1:C:173:PRO:HD2	1:C:199:ALA:HB1	1.99	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	356/375 (95%)	344 (97%)	12 (3%)	0	100	100
1	B	356/375 (95%)	346 (97%)	10 (3%)	0	100	100
1	C	368/375 (98%)	342 (93%)	20 (5%)	6 (2%)	12	8
1	D	368/375 (98%)	340 (92%)	22 (6%)	6 (2%)	12	8
All	All	1448/1500 (96%)	1372 (95%)	64 (4%)	12 (1%)	24	22

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	198	SER
1	D	196	ALA
1	C	196	ALA
1	D	29	SER
1	C	185	GLU
1	D	26	PHE
1	C	147	ALA
1	D	207	ARG
1	C	98	GLY
1	D	147	ALA
1	D	144	GLY
1	C	173	PRO

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	285/297 (96%)	275 (96%)	10 (4%)	43	53
1	B	285/297 (96%)	277 (97%)	8 (3%)	51	63
1	C	294/297 (99%)	272 (92%)	22 (8%)	17	17
1	D	294/297 (99%)	274 (93%)	20 (7%)	20	21
All	All	1158/1188 (98%)	1098 (95%)	60 (5%)	29	33

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	23	LYS
1	A	39	PRO
1	A	89	ASN
1	A	176	ASP
1	A	178	GLN
1	A	185	GLU
1	A	244	LEU
1	A	331	GLU
1	A	370	GLN
1	B	19	ARG
1	B	22	LEU
1	B	68	CYS
1	B	168	LYS
1	B	267	ASN
1	B	299	LEU
1	B	334	LEU
1	B	350	GLN
1	C	22	LEU
1	C	25	ARG
1	C	27	GLU
1	C	136	GLN
1	C	141	VAL
1	C	149	GLU
1	C	150	GLN
1	C	152	THR
1	C	158	ARG
1	C	172	LYS
1	C	175	TRP
1	C	176	ASP
1	C	184	ARG
1	C	185	GLU
1	C	189	ASP

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Mol	Chain	Res	Type
1	C	191	ARG
1	C	207	ARG
1	C	239	ARG
1	C	267	ASN
1	C	287	GLN
1	C	370	GLN
1	C	371	GLU
1	D	6	ARG
1	D	20	LEU
1	D	22	LEU
1	D	28	THR
1	D	56	MET
1	D	89	ASN
1	D	148	ASP
1	D	152	THR
1	D	158	ARG
1	D	172	LYS
1	D	175	TRP
1	D	176	ASP
1	D	184	ARG
1	D	189	ASP
1	D	204	ASP
1	D	208	LEU
1	D	210	GLN
1	D	211	LEU
1	D	239	ARG
1	D	280	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	GLN
1	A	89	ASN
1	A	103	ASN
1	A	150	GLN
1	A	159	HIS
1	A	178	GLN
1	A	221	GLN
1	A	231	HIS
1	A	283	HIS
1	A	287	GLN
1	A	316	ASN

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Mol	Chain	Res	Type
1	B	35	HIS
1	B	221	GLN
1	B	231	HIS
1	B	267	ASN
1	B	283	HIS
1	B	316	ASN
1	B	373	HIS
1	C	33	GLN
1	C	49	GLN
1	C	146	GLN
1	C	197	ASN
1	C	210	GLN
1	C	231	HIS
1	C	267	ASN
1	C	283	HIS
1	C	287	GLN
1	C	310	HIS
1	C	370	GLN
1	D	89	ASN
1	D	103	ASN
1	D	287	GLN
1	D	316	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NLQ	C	1376	-	9,12,12	3.90	4 (44%)	8,15,15	4.02	5 (62%)
3	NLQ	D	2376	-	9,12,12	3.85	4 (44%)	8,15,15	4.17	5 (62%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NLQ	C	1376	-	-	0/9/13/13	0/0/0/0
3	NLQ	D	2376	-	-	1/9/13/13	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	2376	NLQ	C6-N	3.00	1.45	1.34
3	C	1376	NLQ	C6-N	3.05	1.46	1.34
3	C	1376	NLQ	CD-NE2	3.93	1.45	1.32
3	D	2376	NLQ	CD-NE2	4.01	1.45	1.32
3	C	1376	NLQ	OE1-CD	5.94	1.42	1.24
3	D	2376	NLQ	OE1-CD	5.98	1.42	1.24
3	D	2376	NLQ	O4-C6	8.35	1.42	1.23
3	C	1376	NLQ	O4-C6	8.56	1.43	1.23

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2376	NLQ	O4-C6-C7	-7.22	108.82	122.06
3	C	1376	NLQ	O4-C6-C7	-7.07	109.10	122.06
3	D	2376	NLQ	O4-C6-N	-5.48	110.69	121.86
3	D	2376	NLQ	OE1-CD-NE2	-5.35	107.11	122.46
3	C	1376	NLQ	OE1-CD-NE2	-5.10	107.82	122.46
3	C	1376	NLQ	O4-C6-N	-4.96	111.76	121.86
3	D	2376	NLQ	OE1-CD-CG	-3.84	109.86	121.05
3	C	1376	NLQ	C7-C6-N	-3.76	108.90	116.11
3	D	2376	NLQ	C7-C6-N	-3.23	109.93	116.11

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	C	1376	NLQ	OE1-CD-CG	-3.16	111.83	121.05

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	2376	NLQ	O4-C6-N-CA

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1376	NLQ	5	0
3	D	2376	NLQ	2	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, 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	360/375 (96%)	-0.71	0 100 100	11, 18, 36, 49	0
1	B	360/375 (96%)	-0.70	0 100 100	11, 18, 35, 50	0
1	C	370/375 (98%)	-0.28	17 (4%) 36 35	12, 24, 56, 69	0
1	D	370/375 (98%)	-0.27	14 (3%) 44 43	11, 23, 56, 68	0
All	All	1460/1500 (97%)	-0.49	31 (2%) 67 65	11, 21, 52, 69	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	147	ALA	5.7
1	C	175	TRP	4.6
1	D	28	THR	4.6
1	D	175	TRP	3.8
1	D	151	ALA	3.3
1	D	24	PHE	3.3
1	C	188	PRO	3.2
1	C	22	LEU	3.2
1	C	173	PRO	3.1
1	C	35	HIS	3.1
1	D	146	GLN	3.0
1	D	35	HIS	2.7
1	D	152	THR	2.6
1	C	214	TYR	2.6
1	C	174	GLY	2.6
1	D	34	THR	2.6
1	C	145	ILE	2.6
1	C	186	ALA	2.5
1	D	30	PHE	2.5
1	C	34	THR	2.4
1	D	22	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	182	ALA	2.4
1	D	207	ARG	2.3
1	C	185	GLU	2.3
1	C	25	ARG	2.2
1	C	24	PHE	2.2
1	D	186	ALA	2.2
1	D	210	GLN	2.1
1	C	151	ALA	2.1
1	C	26	PHE	2.0
1	D	147	ALA	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	MG	A	1377	1/1	0.98	0.57	35.43	31,31,31,31	0
2	MG	B	2377	1/1	0.98	0.17	5.05	27,27,27,27	0
3	NLQ	C	1376	13/13	0.78	0.32	3.10	43,52,54,54	0
3	NLQ	D	2376	13/13	0.78	0.30	1.87	52,58,59,59	0
2	MG	C	3377	1/1	0.92	0.13	0.17	50,50,50,50	0
2	MG	D	4377	1/1	0.98	0.09	-0.67	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.