



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 02:55 AM GMT

PDB ID : 4JRE  
Title : Crystal structure of nitrate/nitrite exchanger NarK with nitrite bound  
Authors : Zheng, H.; Wisedchaisri, G.; Gonen, T.  
Deposited on : 2013-03-21  
Resolution : 2.80 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

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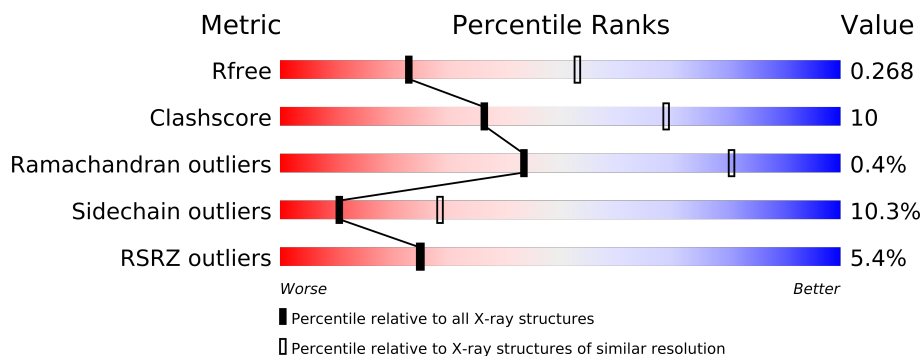
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	466	
1	D	466	
2	B	217	
2	H	217	
3	C	211	
3	L	211	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	NO2	A	501	-	X
4	NO2	D	501	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12589 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Nitrite extrusion protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3088	2055	492	521	20			
1	D	402	Total	C	N	O	S	0	0	0
			3054	2040	484	510	20			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP P10903
A	-1	SER	-	EXPRESSION TAG	UNP P10903
A	0	HIS	-	EXPRESSION TAG	UNP P10903
D	-2	GLY	-	EXPRESSION TAG	UNP P10903
D	-1	SER	-	EXPRESSION TAG	UNP P10903
D	0	HIS	-	EXPRESSION TAG	UNP P10903

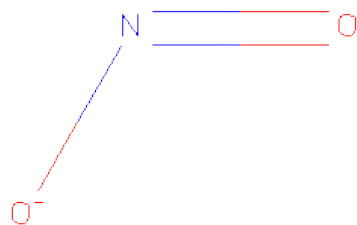
- Molecule 2 is a protein called Immunoglobulin Gamma-2a, Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1594	1017	261	309	7			
2	H	213	Total	C	N	O	S	0	0	0
			1592	1016	261	308	7			

- Molecule 3 is a protein called Immunoglobulin Kappa, Light chain.

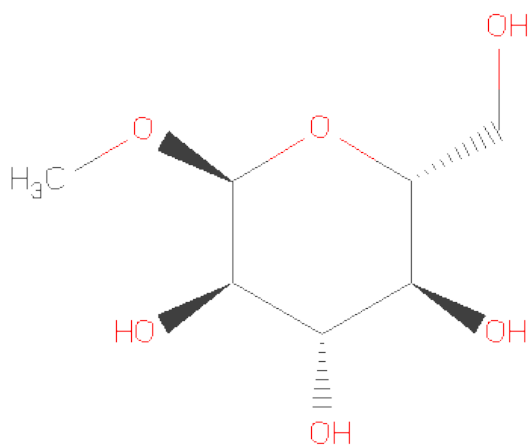
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	211	Total	C	N	O	S	0	0	0
			1597	1002	263	326	6			
3	L	211	Total	C	N	O	S	0	0	0
			1597	1002	262	327	6			

- Molecule 4 is NITRITE ION (three-letter code: NO2) (formula: NO<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	N	O	0	0
			3	1	2		
4	D	1	Total	N	O	0	0
			3	1	2		

- Molecule 5 is SUGAR (METHYL-ALPHA-D-GLUCOPYRANOSIDE) (three-letter code: GYP) (formula: C<sub>7</sub>H<sub>14</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	7	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			13	7	6		

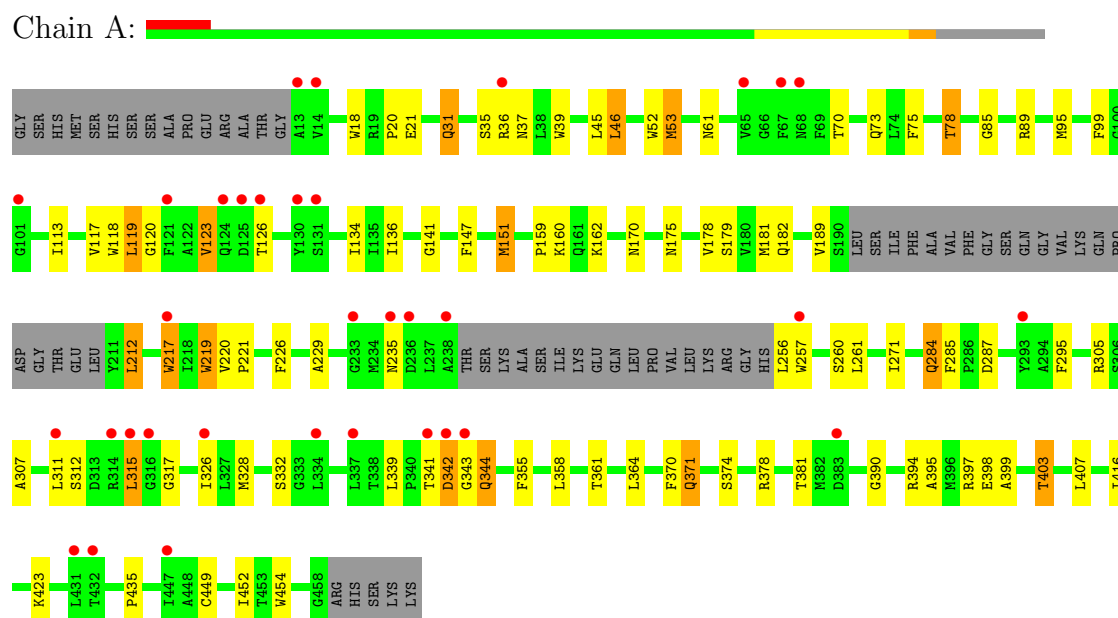
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		
6	B	9	Total	O	0	0
			9	9		
6	C	6	Total	O	0	0
			6	6		
6	D	1	Total	O	0	0
			1	1		
6	H	11	Total	O	0	0
			11	11		
6	L	7	Total	O	0	0
			7	7		

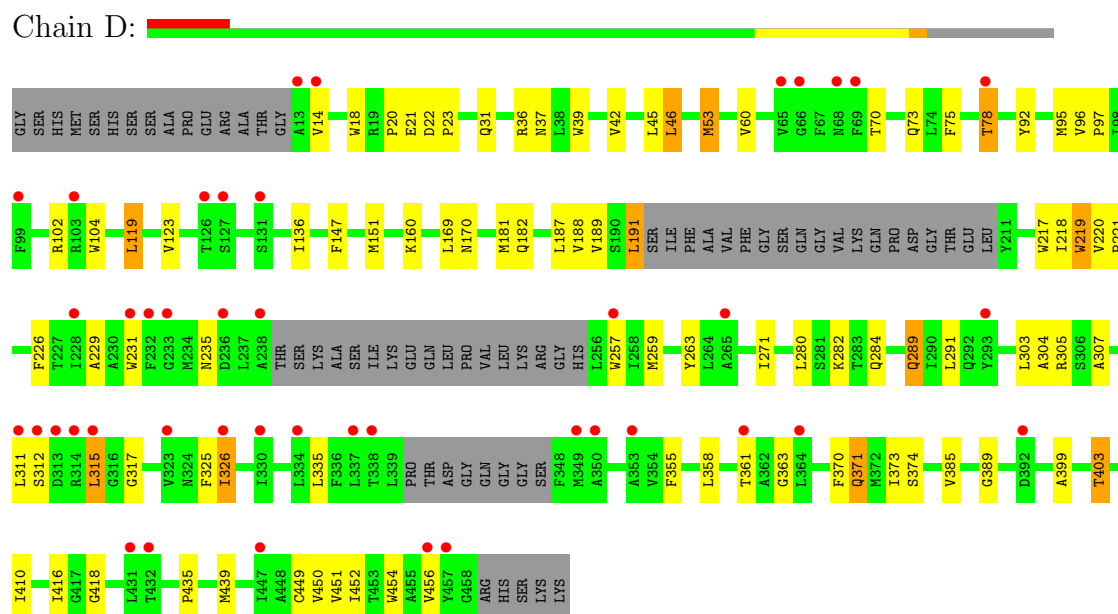
### 3 Residue-property plots

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: Nitrite extrusion protein 1



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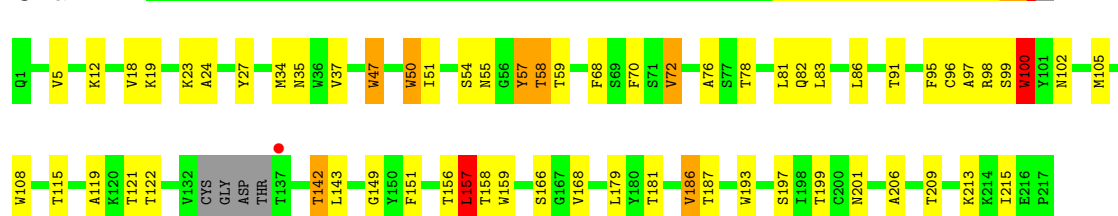
- Molecule 2: Immunoglobulin Gamma-2a, Heavy chain

Chain B:



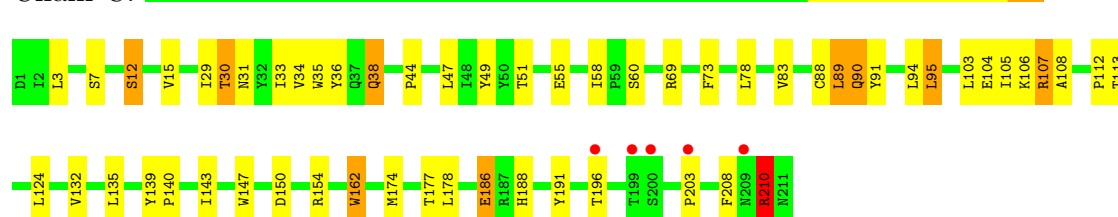
- Molecule 2: Immunoglobulin Gamma-2a, Heavy chain

Chain H:



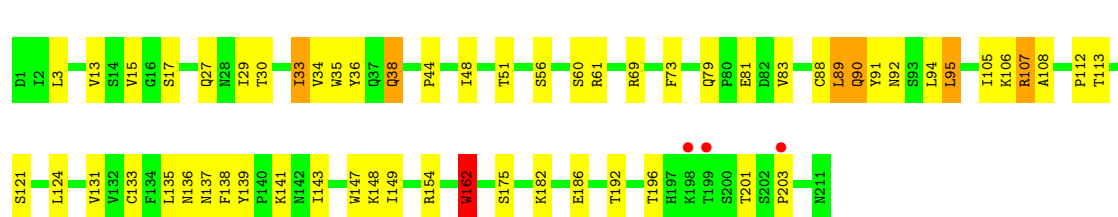
- Molecule 3: Immunoglobulin Kappa, Light chain

Chain C:



- Molecule 3: Immunoglobulin Kappa, Light chain

Chain L:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.91Å 81.41Å 138.49Å 100.07° 96.38° 115.92°	Depositor
Resolution (Å)	50.00 – 2.80 47.04 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.5 (50.00-2.80) 94.6 (47.04-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.223 , 0.269 0.224 , 0.268	Depositor DCC
$R_{free}$ test set	3641 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.7	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 24.0	EDS
Estimated twinning fraction	0.001 for -k,-h,-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 72090 reflections	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	12589	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.



## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NO2, GYP

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	0.53	6/3173 (0.2%)	0.56	2/4312 (0.0%)
1	D	0.53	5/3138 (0.2%)	0.57	2/4263 (0.0%)
2	B	0.65	4/1638 (0.2%)	0.74	2/2237 (0.1%)
2	H	0.65	6/1636 (0.4%)	0.73	1/2234 (0.0%)
3	C	0.54	2/1633 (0.1%)	0.64	1/2230 (0.0%)
3	L	0.54	2/1633 (0.1%)	0.63	1/2230 (0.0%)
All	All	0.56	25/12851 (0.2%)	0.63	9/17506 (0.1%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	162	TRP	CD2-CE2	6.91	1.49	1.41
3	C	162	TRP	CD2-CE2	6.50	1.49	1.41
2	B	100	TRP	CD2-CE2	5.99	1.48	1.41
2	H	100	TRP	CD2-CE2	5.84	1.48	1.41
2	B	159	TRP	CD2-CE2	5.79	1.48	1.41
1	D	39	TRP	CD2-CE2	5.65	1.48	1.41
2	H	159	TRP	CD2-CE2	5.55	1.48	1.41
2	H	50	TRP	CD2-CE2	5.49	1.48	1.41
1	A	39	TRP	CD2-CE2	5.49	1.48	1.41
1	D	217	TRP	CD2-CE2	5.48	1.48	1.41
1	A	454	TRP	CD2-CE2	5.40	1.47	1.41
1	A	219	TRP	CD2-CE2	5.37	1.47	1.41
2	H	108	TRP	CD2-CE2	5.37	1.47	1.41
1	D	454	TRP	CD2-CE2	5.26	1.47	1.41
1	A	217	TRP	CD2-CE2	5.24	1.47	1.41
3	L	147	TRP	CD2-CE2	5.24	1.47	1.41
3	C	147	TRP	CD2-CE2	5.21	1.47	1.41
1	A	52	TRP	CD2-CE2	5.20	1.47	1.41
1	A	257	TRP	CD2-CE2	5.18	1.47	1.41
1	D	219	TRP	CD2-CE2	5.16	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	47	TRP	CD2-CE2	5.13	1.47	1.41
2	B	50	TRP	CD2-CE2	5.13	1.47	1.41
2	H	193	TRP	CD2-CE2	5.12	1.47	1.41
1	D	257	TRP	CD2-CE2	5.09	1.47	1.41
2	B	36	TRP	CD2-CE2	5.07	1.47	1.41

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	315	LEU	CA-CB-CG	6.06	129.23	115.30
2	B	157	LEU	CA-CB-CG	6.00	129.09	115.30
2	H	157	LEU	CA-CB-CG	5.75	128.53	115.30
1	D	46	LEU	CA-CB-CG	5.60	128.17	115.30
1	A	315	LEU	CA-CB-CG	5.47	127.89	115.30
1	A	46	LEU	CA-CB-CG	5.37	127.66	115.30
3	L	95	LEU	CA-CB-CG	5.30	127.49	115.30
3	C	95	LEU	CA-CB-CG	5.24	127.35	115.30
2	B	100	TRP	CA-CB-CG	5.06	123.31	113.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3088	0	3119	49	0
1	D	3054	0	3096	50	0
2	B	1594	0	1546	45	0
2	H	1592	0	1541	47	0
3	C	1597	0	1500	39	0
3	L	1597	0	1498	35	0
4	A	3	0	0	0	0
4	D	3	0	0	0	0
5	A	13	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	13	0	14	0	0
6	A	1	0	0	0	0
6	B	9	0	0	0	0
6	C	6	0	0	0	0
6	D	1	0	0	0	0
6	H	11	0	0	1	0
6	L	7	0	0	1	0
All	All	12589	0	12328	257	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (257) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:100:TRP:HE3	2:B:100:TRP:O	1.39	1.05
2:H:18:VAL:HG23	2:H:86:LEU:HD11	1.43	1.01
1:A:37:ASN:HD21	1:A:235:ASN:HD22	1.04	0.99
2:H:142:THR:HB	2:H:187:THR:HG22	1.47	0.96
2:H:35:ASN:HD22	2:H:47:TRP:HE1	1.13	0.96
2:H:50:TRP:CE2	2:H:100:TRP:HD1	1.84	0.94
1:A:36:ARG:NH2	1:A:235:ASN:HD21	1.64	0.94
2:H:37:VAL:HG21	2:H:105:MET:HE1	1.47	0.93
2:B:50:TRP:CE2	2:B:100:TRP:HD1	1.88	0.92
2:H:100:TRP:O	2:H:100:TRP:HE3	1.52	0.90
1:D:37:ASN:HD21	1:D:235:ASN:HD22	1.20	0.88
1:D:181:MET:HG3	1:D:219:TRP:HH2	1.39	0.86
2:B:37:VAL:CG2	2:B:105:MET:HE1	2.05	0.86
2:H:50:TRP:CE2	2:H:100:TRP:CD1	2.64	0.85
2:B:37:VAL:HG21	2:B:105:MET:HE1	1.56	0.84
2:H:37:VAL:CG2	2:H:105:MET:HE1	2.06	0.84
2:B:100:TRP:CE3	2:B:100:TRP:O	2.28	0.83
2:H:18:VAL:CG2	2:H:86:LEU:HD11	2.08	0.83
2:B:35:ASN:HD22	2:B:47:TRP:HE1	1.27	0.83
1:D:36:ARG:HH21	1:D:235:ASN:HD21	1.25	0.82
1:A:181:MET:HG3	1:A:219:TRP:CH2	2.14	0.81
2:B:34:MET:HE1	2:B:96:CYS:HB2	1.64	0.80
2:B:34:MET:CE	2:B:96:CYS:HB2	2.12	0.79
2:H:76:ALA:O	2:H:78:THR:HG23	1.82	0.79
2:H:50:TRP:CD2	2:H:100:TRP:HD1	2.02	0.78
1:A:399:ALA:O	1:A:403:THR:HG23	1.83	0.77
1:D:36:ARG:NH2	1:D:235:ASN:HD21	1.83	0.76
1:D:326:ILE:HD12	1:D:450:VAL:HG21	1.68	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:50:TRP:CE2	2:B:100:TRP:CD1	2.72	0.76
2:B:35:ASN:ND2	2:B:47:TRP:HE1	1.84	0.75
2:B:100:TRP:HZ3	3:C:91:TYR:O	1.70	0.75
1:A:36:ARG:HH21	1:A:235:ASN:HD21	1.33	0.75
2:H:100:TRP:O	2:H:100:TRP:CE3	2.39	0.75
2:H:142:THR:HB	2:H:187:THR:CG2	2.20	0.72
1:D:312:SER:OG	1:D:317:GLY:HA2	1.91	0.70
1:A:37:ASN:ND2	1:A:235:ASN:HD22	1.86	0.70
1:D:119:LEU:HB3	1:D:136:ILE:HG21	1.74	0.69
2:B:50:TRP:CD2	2:B:100:TRP:HD1	2.11	0.69
2:B:51:ILE:HD13	2:B:72:VAL:HG23	1.75	0.69
2:B:76:ALA:O	2:B:78:THR:HG23	1.93	0.68
1:A:119:LEU:HB3	1:A:136:ILE:HG21	1.76	0.68
1:D:181:MET:HG3	1:D:219:TRP:CH2	2.26	0.68
1:D:399:ALA:O	1:D:403:THR:HG23	1.94	0.66
3:L:148:LYS:HB2	3:L:192:THR:HB	1.78	0.66
3:C:196:THR:HG22	3:C:203:PRO:HB3	1.78	0.65
2:H:100:TRP:HZ3	3:L:91:TYR:O	1.79	0.65
2:B:100:TRP:CZ3	3:C:91:TYR:O	2.49	0.65
3:L:34:VAL:HG23	3:L:89:LEU:HB3	1.77	0.64
2:H:35:ASN:ND2	2:H:47:TRP:HE1	1.90	0.64
3:C:106:LYS:HE3	2:H:206:ALA:O	1.99	0.62
2:H:55:ASN:HB3	2:H:57:TYR:HB2	1.81	0.62
1:D:18:TRP:NE1	1:D:20:PRO:HG3	2.15	0.62
3:C:38:GLN:HG3	3:C:44:PRO:HG3	1.82	0.61
2:B:97:ALA:HB3	2:B:105:MET:HE2	1.82	0.61
2:B:58:THR:HG22	2:B:70:PHE:HB2	1.83	0.61
3:C:112:PRO:HG3	3:C:143:ILE:HD11	1.83	0.60
3:L:38:GLN:HG3	3:L:44:PRO:HG3	1.85	0.59
1:D:191:LEU:H	1:D:191:LEU:HD22	1.67	0.59
1:D:358:LEU:HA	1:D:361:THR:HG22	1.82	0.59
2:H:34:MET:CE	2:H:96:CYS:HB2	2.32	0.59
1:A:182:GLN:HE21	1:A:295:PHE:HA	1.66	0.59
2:B:37:VAL:HG23	2:B:105:MET:HE1	1.84	0.59
3:L:33:ILE:HG22	3:L:51:THR:HA	1.84	0.58
2:B:142:THR:HG22	2:B:187:THR:HB	1.84	0.58
2:H:98:ARG:O	2:H:105:MET:HA	2.03	0.58
3:L:35:TRP:CH2	3:L:88:CYS:HB3	2.38	0.58
1:A:358:LEU:HA	1:A:361:THR:HG22	1.85	0.58
3:L:162:TRP:N	3:L:162:TRP:CD1	2.72	0.58
1:A:123:VAL:HG21	1:A:212:LEU:HD12	1.86	0.57
3:C:29:ILE:HG21	3:C:90:GLN:HG3	1.87	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:143:LEU:HD22	2:H:215:ILE:HG21	1.86	0.57
2:B:18:VAL:HG22	2:B:86:LEU:HD11	1.85	0.57
1:D:53:MET:CE	1:D:53:MET:HA	2.34	0.56
2:H:168:VAL:HG22	2:H:186:VAL:CG1	2.35	0.56
1:D:21:GLU:OE2	1:D:160:LYS:HG2	2.05	0.56
1:A:307:ALA:O	1:A:311:LEU:HB2	2.05	0.56
1:D:188:VAL:HG21	1:D:218:ILE:HD12	1.88	0.56
1:A:18:TRP:NE1	1:A:20:PRO:HG3	2.21	0.56
3:L:34:VAL:HG13	3:L:91:TYR:CE1	2.41	0.56
2:H:91:THR:HG23	2:H:115:THR:HA	1.88	0.56
3:C:34:VAL:HG12	3:C:49:TYR:HA	1.88	0.56
1:D:181:MET:HE2	1:D:182:GLN:HG3	1.88	0.55
3:C:94:LEU:O	3:C:95:LEU:HD23	2.05	0.55
2:H:157:LEU:HD12	2:H:158:THR:N	2.22	0.55
2:H:100:TRP:CZ3	3:L:91:TYR:O	2.58	0.55
3:C:35:TRP:CZ3	3:C:88:CYS:HB3	2.42	0.55
2:H:50:TRP:CD2	2:H:100:TRP:CD1	2.89	0.55
2:H:34:MET:HE1	2:H:96:CYS:HB2	1.89	0.55
2:B:175:LEU:HB2	2:B:180:TYR:CE1	2.42	0.55
3:C:33:ILE:HG22	3:C:51:THR:HA	1.89	0.55
1:A:75:PHE:O	1:A:78:THR:HG22	2.07	0.54
3:L:196:THR:HG22	3:L:203:PRO:HB3	1.90	0.54
1:D:325:PHE:CE2	1:D:449:CYS:HB3	2.43	0.54
2:B:159:TRP:CE2	2:B:186:VAL:HG22	2.43	0.54
3:C:143:ILE:HG22	3:C:162:TRP:CZ3	2.43	0.54
3:C:35:TRP:CE2	3:C:73:PHE:HB2	2.43	0.54
3:C:35:TRP:CH2	3:C:88:CYS:HB3	2.43	0.53
3:L:107:ARG:HD2	3:L:139:TYR:CB	2.38	0.53
1:A:181:MET:CG	1:A:219:TRP:CH2	2.90	0.53
1:A:312:SER:OG	1:A:317:GLY:HA2	2.09	0.53
2:B:97:ALA:HB3	2:B:105:MET:CE	2.39	0.53
2:B:34:MET:HE1	2:B:96:CYS:CB	2.37	0.53
3:L:106:LYS:HA	3:L:139:TYR:OH	2.09	0.53
2:B:91:THR:HG23	2:B:115:THR:HA	1.90	0.52
3:C:34:VAL:HG13	3:C:91:TYR:CE1	2.44	0.52
2:B:157:LEU:HD12	2:B:157:LEU:C	2.30	0.52
3:L:143:ILE:HG22	3:L:162:TRP:CZ3	2.45	0.52
1:A:381:THR:HG21	1:A:398:GLU:HB2	1.92	0.52
1:D:147:PHE:O	1:D:151:MET:HB2	2.09	0.52
3:L:143:ILE:HG22	3:L:162:TRP:CH2	2.45	0.52
1:D:312:SER:HG	1:D:317:GLY:HA2	1.75	0.52
2:H:50:TRP:CZ2	2:H:100:TRP:CD1	2.98	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:181:MET:CE	1:A:182:GLN:HG3	2.41	0.51
2:B:168:VAL:HG22	2:B:186:VAL:HG13	1.91	0.51
1:D:60:VAL:HG11	1:D:291:LEU:HD11	1.92	0.51
1:A:151:MET:HG2	1:A:407:LEU:HD21	1.92	0.51
3:C:12:SER:HB2	3:C:106:LYS:HE2	1.93	0.51
2:B:68:PHE:CE2	2:B:83:LEU:HD21	2.45	0.51
3:C:154:ARG:HG2	3:C:178:LEU:HD11	1.93	0.51
1:D:75:PHE:O	1:D:78:THR:HG22	2.11	0.51
1:D:325:PHE:CD2	1:D:449:CYS:HB3	2.47	0.50
3:C:12:SER:HA	3:C:104:GLU:O	2.11	0.50
3:L:35:TRP:CZ3	3:L:88:CYS:HB3	2.46	0.50
1:A:449:CYS:HA	1:A:452:ILE:HG22	1.94	0.50
3:C:91:TYR:HA	3:C:95:LEU:HD22	1.93	0.50
1:A:312:SER:HB3	1:A:371:GLN:HG2	1.94	0.50
2:H:37:VAL:CG2	2:H:105:MET:CE	2.85	0.50
3:L:182:LYS:O	3:L:186:GLU:HB2	2.12	0.50
1:A:118:TRP:CE3	1:A:136:ILE:HG12	2.46	0.50
2:H:68:PHE:CE2	2:H:83:LEU:HD23	2.47	0.50
3:C:143:ILE:HG22	3:C:162:TRP:CH2	2.47	0.49
2:H:58:THR:HG22	2:H:70:PHE:HB2	1.94	0.49
1:D:373:ILE:HD13	1:D:410:ILE:HD13	1.94	0.49
3:L:112:PRO:HG3	3:L:143:ILE:HD11	1.93	0.49
3:C:186:GLU:O	3:C:210:ARG:NH2	2.45	0.49
3:L:107:ARG:HD3	3:L:108:ALA:O	2.12	0.49
1:D:263:TYR:OH	1:D:305:ARG:NH2	2.46	0.49
3:C:89:LEU:HD21	3:C:95:LEU:HD13	1.95	0.49
1:D:37:ASN:ND2	1:D:235:ASN:HD22	2.00	0.49
2:H:157:LEU:C	2:H:157:LEU:HD12	2.32	0.49
3:L:89:LEU:HD21	3:L:95:LEU:HD13	1.94	0.49
3:L:94:LEU:O	3:L:95:LEU:HD23	2.13	0.49
1:A:160:LYS:HG3	1:A:397:ARG:HG2	1.94	0.49
2:H:51:ILE:HD13	2:H:72:VAL:HG23	1.95	0.48
1:D:271:ILE:HG22	1:D:418:GLY:HA3	1.94	0.48
1:A:120:GLY:HA3	1:A:217:TRP:NE1	2.27	0.48
2:H:12:LYS:HG3	2:H:18:VAL:HG22	1.95	0.48
3:C:150:ASP:OD2	3:C:188:HIS:HB3	2.14	0.48
1:A:159:PRO:HG2	1:A:162:LYS:HB2	1.96	0.48
3:C:34:VAL:HG21	3:C:36:TYR:OH	2.13	0.48
2:H:55:ASN:HB3	2:H:57:TYR:H	1.78	0.48
1:A:226:PHE:HA	1:A:229:ALA:HB3	1.94	0.48
2:B:13:LYS:HG3	2:B:16:GLN:NE2	2.29	0.47
2:B:119:ALA:HB3	2:B:151:PHE:CZ	2.50	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:31:GLN:O	1:A:35:SER:HB3	2.13	0.47
3:L:83:VAL:HG21	6:L:302:HOH:O	2.12	0.47
2:H:50:TRP:CZ2	2:H:100:TRP:HD1	2.28	0.47
3:C:107:ARG:HD3	3:C:108:ALA:O	2.15	0.47
1:A:175:ASN:ND2	1:A:305:ARG:HH11	2.12	0.47
1:D:181:MET:CG	1:D:219:TRP:HH2	2.20	0.47
2:B:128:PRO:HD3	2:B:213:LYS:HG2	1.96	0.47
1:D:70:THR:HB	1:D:73:GLN:H	1.79	0.47
3:C:34:VAL:CG2	3:C:89:LEU:HD23	2.44	0.47
1:D:449:CYS:HA	1:D:452:ILE:HG22	1.97	0.47
3:L:34:VAL:HG21	3:L:36:TYR:OH	2.15	0.47
2:H:37:VAL:HB	2:H:95:PHE:HB2	1.96	0.47
3:L:35:TRP:CE2	3:L:73:PHE:HB2	2.49	0.47
1:D:53:MET:HE3	1:D:53:MET:HA	1.97	0.47
2:H:97:ALA:HB3	2:H:105:MET:HE2	1.97	0.46
2:H:119:ALA:HB3	2:H:151:PHE:CE2	2.50	0.46
1:D:96:VAL:HB	1:D:97:PRO:HD3	1.98	0.46
1:A:45:LEU:HD23	1:A:170:ASN:O	2.15	0.46
1:A:371:GLN:HA	1:A:374:SER:HB3	1.96	0.46
3:C:47:LEU:HA	3:C:58:ILE:HG13	1.96	0.46
1:D:226:PHE:HA	1:D:229:ALA:HB3	1.98	0.46
2:B:48:MET:HG2	2:B:64:PHE:CE1	2.51	0.46
2:H:50:TRP:CD1	2:H:59:THR:HB	2.50	0.46
2:B:37:VAL:HG23	2:B:105:MET:CE	2.45	0.46
1:A:390:GLY:HA3	1:A:394:ARG:NH2	2.31	0.46
1:A:343:GLY:HA2	1:A:344:GLN:HA	1.69	0.46
1:A:381:THR:HG22	1:A:395:ALA:HA	1.98	0.46
2:B:52:ASN:HB3	2:B:55:ASN:OD1	2.16	0.46
3:L:91:TYR:CB	3:L:95:LEU:HD22	2.45	0.45
2:B:39:GLN:HE22	3:C:38:GLN:HE22	1.64	0.45
3:L:138:PHE:HE2	3:L:141:LYS:O	1.99	0.45
2:B:48:MET:HA	2:B:64:PHE:CD2	2.52	0.45
2:B:152:PRO:HD2	2:B:206:ALA:CB	2.46	0.45
2:B:212:ASP:O	2:B:213:LYS:HD2	2.17	0.45
2:H:142:THR:CB	2:H:187:THR:HG22	2.31	0.45
2:H:68:PHE:HE2	2:H:83:LEU:HD23	1.81	0.45
1:A:339:LEU:HD13	1:A:435:PRO:HG2	1.99	0.44
3:L:91:TYR:HA	3:L:95:LEU:HD22	1.98	0.44
2:H:47:TRP:CE2	3:L:95:LEU:HG	2.53	0.44
1:D:312:SER:HB3	1:D:371:GLN:HG2	1.99	0.44
3:C:55:GLU:HA	3:C:55:GLU:OE1	2.18	0.44
1:A:21:GLU:OE2	1:A:160:LYS:HG2	2.18	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:132:VAL:HG22	3:C:177:THR:HG22	2.00	0.44
2:B:50:TRP:CD1	2:B:59:THR:HB	2.53	0.44
1:A:378:ARG:HG3	1:A:399:ALA:HB1	1.98	0.44
2:H:149:GLY:HA2	2:H:179:LEU:HB3	1.99	0.44
2:B:34:MET:HE2	2:B:96:CYS:HB2	1.95	0.44
2:B:51:ILE:CD1	2:B:72:VAL:HG23	2.46	0.43
1:A:85:GLY:O	1:A:89:ARG:HG3	2.18	0.43
3:C:191:TYR:HB2	3:C:208:PHE:CE2	2.53	0.43
2:H:23:LYS:HA	2:H:78:THR:HG22	2.01	0.43
2:B:175:LEU:HD13	2:B:180:TYR:CE2	2.53	0.43
1:D:307:ALA:O	1:D:311:LEU:HB2	2.19	0.43
1:A:147:PHE:O	1:A:151:MET:HB2	2.19	0.43
3:C:94:LEU:C	3:C:95:LEU:HD23	2.39	0.43
3:L:34:VAL:HA	3:L:48:ILE:O	2.19	0.42
2:B:189:THR:OG1	2:B:192:THR:HG22	2.18	0.42
1:D:385:VAL:O	1:D:389:GLY:N	2.48	0.42
2:H:19:LYS:HA	2:H:81:LEU:O	2.19	0.42
1:D:102:ARG:HD2	1:D:231:TRP:O	2.19	0.42
3:C:33:ILE:CG2	3:C:51:THR:HA	2.50	0.42
1:D:335:LEU:HD23	1:D:439:MET:SD	2.59	0.42
1:A:220:VAL:N	1:A:221:PRO:HD2	2.35	0.42
2:H:70:PHE:HB3	6:H:303:HOH:O	2.19	0.42
1:D:435:PRO:O	1:D:439:MET:HB2	2.19	0.42
3:L:149:ILE:HD12	3:L:154:ARG:HD3	2.00	0.42
1:A:36:ARG:HH21	1:A:235:ASN:ND2	2.10	0.42
1:A:85:GLY:HA2	1:A:141:GLY:O	2.20	0.42
1:D:220:VAL:N	1:D:221:PRO:HD2	2.35	0.42
2:B:48:MET:HG2	2:B:64:PHE:CZ	2.54	0.42
1:A:341:THR:O	1:A:343:GLY:HA2	2.20	0.42
1:A:423:LYS:HD2	1:A:423:LYS:HA	1.86	0.42
1:D:280:LEU:C	1:D:282:LYS:H	2.23	0.42
3:L:34:VAL:CG2	3:L:89:LEU:HB3	2.46	0.42
1:D:304:ALA:HB3	1:D:363:GLY:HA3	2.02	0.42
3:L:89:LEU:HG	3:L:90:GLN:N	2.35	0.41
1:A:53:MET:HG2	1:A:178:VAL:HG13	2.02	0.41
1:A:284:GLN:HB3	1:A:285:PHE:CD1	2.55	0.41
1:D:259:MET:CE	1:D:259:MET:HA	2.50	0.41
1:D:92:TYR:HA	1:D:95:MET:HG2	2.02	0.41
1:D:95:MET:HG3	1:D:104:TRP:CZ2	2.56	0.41
3:L:29:ILE:HG21	3:L:90:GLN:HG3	2.01	0.41
3:L:136:ASN:HB3	3:L:137:ASN:OD1	2.20	0.41
3:C:29:ILE:CG2	3:C:90:GLN:HG3	2.50	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:70:THR:HB	1:A:73:GLN:H	1.86	0.41
1:A:95:MET:HE3	1:A:99:PHE:HE2	1.85	0.41
1:D:271:ILE:HA	1:D:271:ILE:HD13	1.91	0.41
1:A:342:ASP:HA	1:A:343:GLY:HA3	1.94	0.41
3:C:139:TYR:CD1	3:C:140:PRO:HA	2.55	0.41
3:L:38:GLN:CG	3:L:44:PRO:HG3	2.50	0.41
1:D:456:VAL:HG12	1:D:456:VAL:O	2.21	0.41
1:D:289:GLN:HB3	1:D:289:GLN:HE21	1.75	0.41
3:L:13:VAL:CG1	3:L:17:SER:CB	2.99	0.41
1:D:45:LEU:HD11	1:D:147:PHE:HA	2.03	0.41
3:C:139:TYR:CG	3:C:140:PRO:HA	2.56	0.41
3:C:78:LEU:HD11	3:C:103:LEU:HD21	2.03	0.41
2:H:24:ALA:HB1	2:H:27:TYR:CE1	2.56	0.41
1:D:22:ASP:HA	1:D:23:PRO:HD2	1.94	0.40
1:A:61:ASN:CB	1:A:212:LEU:HD21	2.51	0.40
1:A:113:ILE:O	1:A:117:VAL:HG23	2.22	0.40
1:D:42:VAL:HG22	1:D:170:ASN:HA	2.04	0.40
2:B:108:TRP:CE2	3:C:44:PRO:HB2	2.57	0.40
3:C:30:THR:O	3:C:31:ASN:HB2	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	403/466 (86%)	384 (95%)	18 (4%)	1 (0%)	56	88
1	D	394/466 (84%)	377 (96%)	17 (4%)	0	100	100
2	B	209/217 (96%)	197 (94%)	10 (5%)	2 (1%)	22	60
2	H	209/217 (96%)	200 (96%)	8 (4%)	1 (0%)	38	76
3	C	209/211 (99%)	193 (92%)	15 (7%)	1 (0%)	38	76
3	L	209/211 (99%)	197 (94%)	11 (5%)	1 (0%)	38	76
All	All	1633/1788 (91%)	1548 (95%)	79 (5%)	6 (0%)	43	80

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	99	SER
1	A	342	ASP
3	C	210	ARG
2	H	99	SER
3	L	92	ASN
2	B	55	ASN

### 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	314/364 (86%)	285 (91%)	29 (9%)	13	36
1	D	311/364 (85%)	288 (93%)	23 (7%)	20	48
2	B	175/182 (96%)	155 (89%)	20 (11%)	8	24
2	H	174/182 (96%)	153 (88%)	21 (12%)	7	21
3	C	178/190 (94%)	159 (89%)	19 (11%)	10	26
3	L	178/190 (94%)	153 (86%)	25 (14%)	5	15
All	All	1330/1472 (90%)	1193 (90%)	137 (10%)	10	28

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	46	LEU
1	A	53	MET
1	A	78	THR
1	A	119	LEU
1	A	123	VAL
1	A	126	THR
1	A	134	ILE
1	A	151	MET
1	A	179	SER
1	A	189	VAL
1	A	212	LEU
1	A	256	LEU

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Mol	Chain	Res	Type
1	A	260	SER
1	A	261	LEU
1	A	271	ILE
1	A	284	GLN
1	A	287	ASP
1	A	315	LEU
1	A	326	ILE
1	A	328	MET
1	A	332	SER
1	A	344	GLN
1	A	355	PHE
1	A	364	LEU
1	A	370	PHE
1	A	371	GLN
1	A	403	THR
1	A	416	ILE
2	B	18	VAL
2	B	57	TYR
2	B	58	THR
2	B	83	LEU
2	B	98	ARG
2	B	100	TRP
2	B	102	ASN
2	B	113	SER
2	B	121	THR
2	B	142	THR
2	B	148	LYS
2	B	157	LEU
2	B	181	THR
2	B	185	SER
2	B	186	VAL
2	B	187	THR
2	B	192	THR
2	B	195	SER
2	B	201	ASN
2	B	209	THR
3	C	3	LEU
3	C	7	SER
3	C	12	SER
3	C	15	VAL
3	C	30	THR
3	C	38	GLN

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Mol	Chain	Res	Type
3	C	60	SER
3	C	69	ARG
3	C	83	VAL
3	C	89	LEU
3	C	90	GLN
3	C	105	ILE
3	C	107	ARG
3	C	113	THR
3	C	124	LEU
3	C	135	LEU
3	C	174	MET
3	C	186	GLU
3	C	210	ARG
1	D	14	VAL
1	D	31	GLN
1	D	46	LEU
1	D	53	MET
1	D	78	THR
1	D	119	LEU
1	D	123	VAL
1	D	169	LEU
1	D	187	LEU
1	D	189	VAL
1	D	191	LEU
1	D	284	GLN
1	D	289	GLN
1	D	303	LEU
1	D	315	LEU
1	D	326	ILE
1	D	355	PHE
1	D	370	PHE
1	D	371	GLN
1	D	374	SER
1	D	403	THR
1	D	416	ILE
1	D	451	VAL
2	H	5	VAL
2	H	54	SER
2	H	57	TYR
2	H	58	THR
2	H	72	VAL
2	H	82	GLN

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Mol	Chain	Res	Type
2	H	100	TRP
2	H	102	ASN
2	H	121	THR
2	H	122	THR
2	H	142	THR
2	H	156	THR
2	H	157	LEU
2	H	166	SER
2	H	181	THR
2	H	186	VAL
2	H	197	SER
2	H	199	THR
2	H	201	ASN
2	H	209	THR
2	H	213	LYS
3	L	3	LEU
3	L	15	VAL
3	L	27	GLN
3	L	30	THR
3	L	33	ILE
3	L	38	GLN
3	L	56	SER
3	L	60	SER
3	L	61	ARG
3	L	69	ARG
3	L	79	GLN
3	L	81	GLU
3	L	89	LEU
3	L	90	GLN
3	L	105	ILE
3	L	107	ARG
3	L	113	THR
3	L	121	SER
3	L	124	LEU
3	L	131	VAL
3	L	133	CYS
3	L	135	LEU
3	L	162	TRP
3	L	175	SER
3	L	201	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	163	GLN
1	A	175	ASN
1	A	182	GLN
1	A	235	ASN
2	B	35	ASN
2	B	39	GLN
3	C	38	GLN
3	C	197	HIS
1	D	163	GLN
1	D	182	GLN
1	D	235	ASN
1	D	284	GLN
1	D	289	GLN
2	H	35	ASN
2	H	39	GLN
3	L	38	GLN
3	L	197	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

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
4	NO2	A	501	-	2,2,2	0.93	0	1,1,1	0.22	0
5	GYP	A	502	-	13,13,13	0.77	1 (7%)	18,18,18	1.43	2 (11%)
4	NO2	D	501	-	2,2,2	0.93	0	1,1,1	0.18	0
5	GYP	D	502	-	13,13,13	0.80	1 (7%)	18,18,18	1.42	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NO2	A	501	-	-	0/0/0/0	0/0/0/0
5	GYP	A	502	-	-	0/4/24/24	0/1/1/1
4	NO2	D	501	-	-	0/0/0/0	0/0/0/0
5	GYP	D	502	-	-	0/4/24/24	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	502	GYP	O1-C1	2.37	1.44	1.40
5	A	502	GYP	O1-C1	2.33	1.44	1.40

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	502	GYP	O1-C1-C2	4.66	113.89	108.18
5	D	502	GYP	O1-C1-C2	4.36	113.52	108.18
5	A	502	GYP	C1-C2-C3	2.66	115.17	110.00
5	D	502	GYP	C1-O5-C5	2.63	118.84	113.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	409/466 (87%)	0.21	34 (8%) 11 10	30, 73, 105, 139	0
1	D	402/466 (86%)	0.48	43 (10%) 6 6	30, 78, 105, 125	0
2	B	213/217 (98%)	-0.39	0 100 100	23, 36, 62, 112	0
2	H	213/217 (98%)	-0.46	1 (0%) 88 90	24, 35, 63, 94	0
3	C	211/211 (100%)	-0.34	5 (2%) 56 57	25, 41, 69, 84	0
3	L	211/211 (100%)	-0.37	3 (1%) 72 72	23, 40, 70, 84	0
All	All	1659/1788 (92%)	-0.03	86 (5%) 25 26	23, 53, 100, 139	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	314	ARG	8.0
1	D	315	LEU	7.1
1	D	431	LEU	6.7
1	A	65	VAL	6.4
1	D	311	LEU	6.3
1	A	315	LEU	5.3
1	A	68	ASN	5.2
1	D	337	LEU	5.0
1	D	364	LEU	5.0
1	A	343	GLY	4.8
1	D	127	SER	4.7
1	D	13	ALA	4.7
1	A	13	ALA	4.7
1	D	68	ASN	4.6
1	D	126	THR	4.5
1	D	350	ALA	4.4
1	D	334	LEU	4.1
1	D	456	VAL	4.0
1	A	131	SER	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	313	ASP	3.8
1	D	349	MET	3.8
1	A	314	ARG	3.6
1	D	131	SER	3.6
3	C	209	ASN	3.5
1	D	432	THR	3.5
1	D	457	TYR	3.5
3	L	199	THR	3.4
1	A	36	ARG	3.4
1	D	257	TRP	3.4
1	D	236	ASP	3.3
1	A	235	ASN	3.3
1	A	342	ASP	3.3
1	A	257	TRP	3.2
1	D	312	SER	3.2
1	D	361	THR	3.2
1	D	99	PHE	3.1
1	D	238	ALA	3.1
1	A	238	ALA	3.1
1	A	121	PHE	3.0
1	A	126	THR	3.0
1	D	326	ILE	3.0
3	C	199	THR	3.0
1	A	337	LEU	3.0
1	A	431	LEU	2.9
1	D	265	ALA	2.9
1	D	330	ILE	2.9
1	A	125	ASP	2.9
1	A	217	TRP	2.9
1	A	316	GLY	2.8
1	D	353	ALA	2.8
1	A	236	ASP	2.8
1	D	231	TRP	2.8
1	D	65	VAL	2.7
1	A	101	GLY	2.7
1	D	293	TYR	2.7
1	A	293	TYR	2.6
1	D	232	PHE	2.6
3	C	203	PRO	2.6
1	A	341	THR	2.5
1	A	447	ILE	2.5
1	D	14	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	383	ASP	2.4
1	D	323	VAL	2.4
2	H	137	THR	2.4
1	A	130	TYR	2.4
1	D	78	THR	2.4
1	A	124	GLN	2.4
1	A	326	ILE	2.4
3	C	200	SER	2.3
3	L	203	PRO	2.3
1	D	228	ILE	2.3
1	A	14	VAL	2.3
1	D	103	ARG	2.3
1	D	392	ASP	2.3
1	D	447	ILE	2.2
3	C	196	THR	2.2
1	D	233	GLY	2.2
1	A	311	LEU	2.1
1	D	69	PHE	2.1
1	A	432	THR	2.1
1	D	338	THR	2.1
3	L	198	LYS	2.1
1	A	334	LEU	2.1
1	A	67	PHE	2.1
1	A	233	GLY	2.0
1	D	66	GLY	2.0

## 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 carbohydrates 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. 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, 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NO2	D	501	3/3	0.95	35.39	71,71,72,73	0
4	NO2	A	501	3/3	0.47	16.88	78,78,80,80	0
5	GYP	A	502	13/13	0.18	0.42	82,91,99,106	0
5	GYP	D	502	13/13	0.20	0.06	86,96,108,119	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.