



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 09:39 PM BST

PDB ID : 2QFP  
Title : Crystal structure of red kidney bean purple acid phosphatase in complex with fluoride  
Authors : Guddat, L.W.; Schenk, G.S.; Gahan, L.R.; Elliot, T.W.; Leung, E.  
Deposited on : 2007-06-27  
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](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.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
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) : 2.13.1

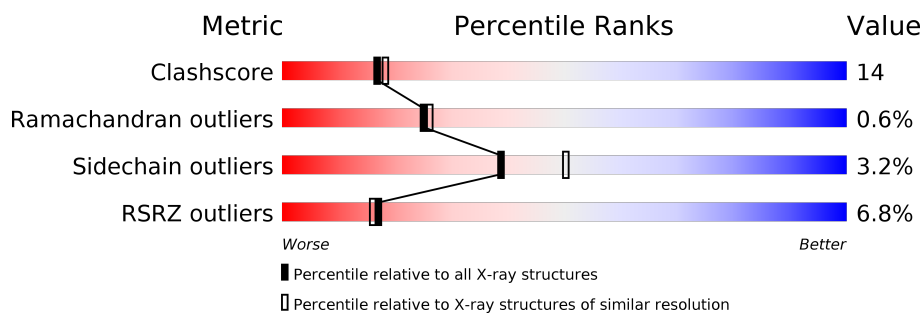
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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  $\geq 3$ , 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	424	<div> <div>6%</div> <div> <div></div> <div>73%</div> <div>25%</div> <div>.</div> </div> </div>
1	B	424	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>24%</div> <div>.</div> </div> </div>
1	C	424	<div> <div>9%</div> <div> <div></div> <div>73%</div> <div>25%</div> <div>.</div> </div> </div>
1	D	424	<div> <div>7%</div> <div> <div></div> <div>68%</div> <div>29%</div> <div>.</div> </div> </div>

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
6	NAG	B	438	X	-	-	-
6	NAG	B	439	X	-	-	-
6	NAG	C	439	X	-	-	-
6	NAG	D	440	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 14782 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 Purple acid phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	424	Total	C	N	O	S	0	0	0
			3487	2240	603	634	10			
1	B	424	Total	C	N	O	S	0	0	0
			3487	2240	603	634	10			
1	C	424	Total	C	N	O	S	0	0	0
			3487	2240	603	634	10			
1	D	424	Total	C	N	O	S	0	0	0
			3487	2240	603	634	10			

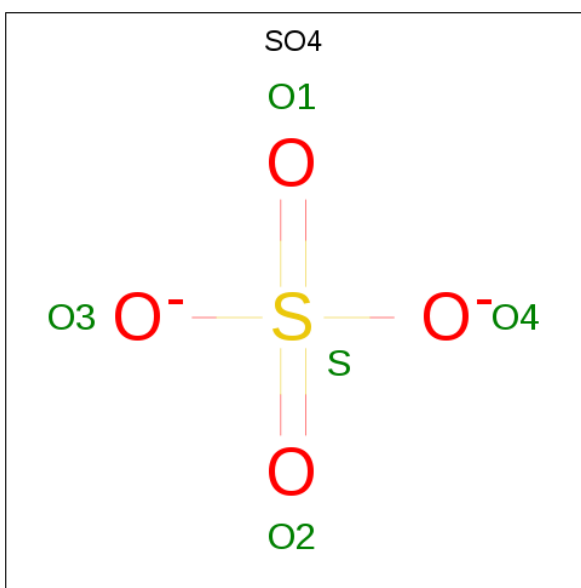
- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is FLUORIDE ION (three-letter code: F) (formula: F).

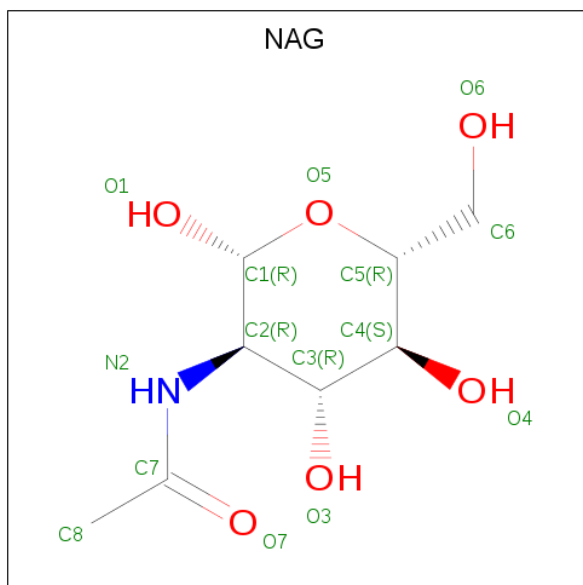
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	F	0	0
			1	1		
5	A	1	Total	F	0	0
			1	1		
5	D	1	Total	F	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	F	0	0
			1	1		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	3	Total	Na	0	0
			3	3		
7	A	3	Total	Na	0	0
			3	3		
7	D	2	Total	Na	0	0
			2	2		
7	C	3	Total	Na	0	0
			3	3		

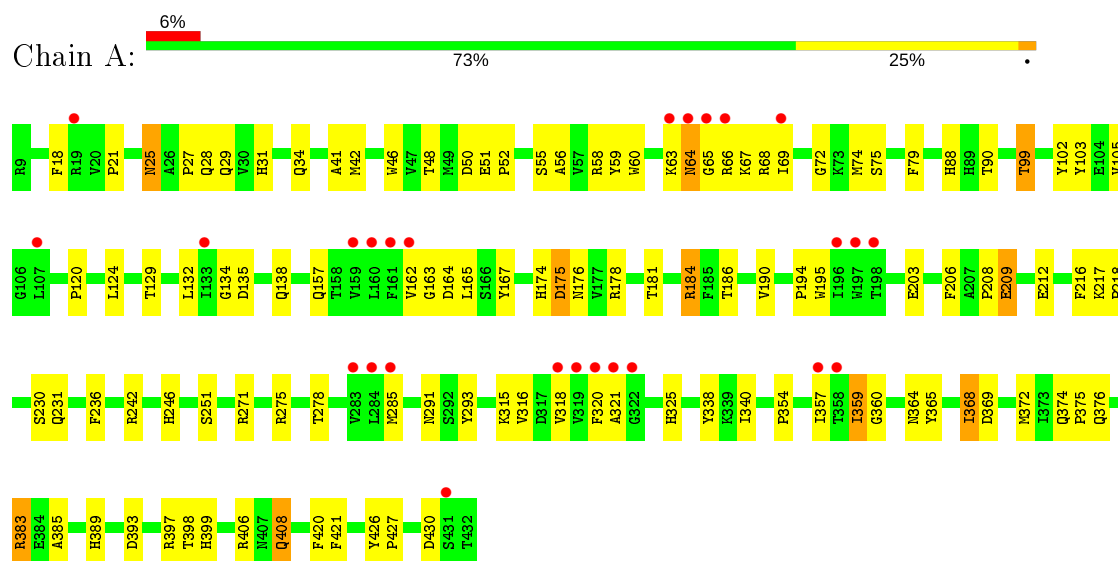
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	150	Total	O	0	0
			150	150		
8	B	168	Total	O	0	0
			168	168		
8	C	105	Total	O	0	0
			105	105		
8	D	124	Total	O	0	0
			124	124		

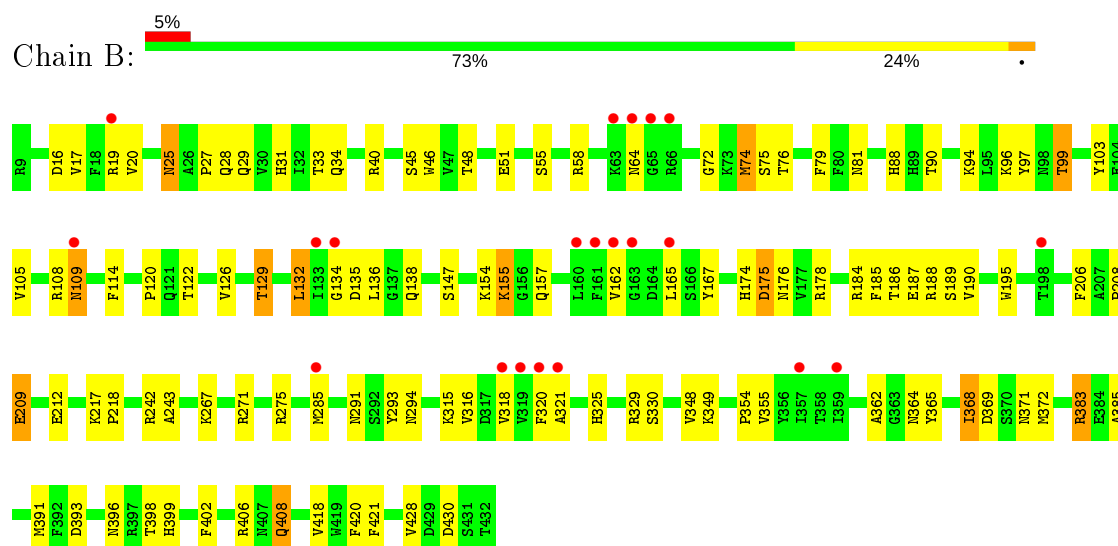
### 3 Residue-property plots [i](#)

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.

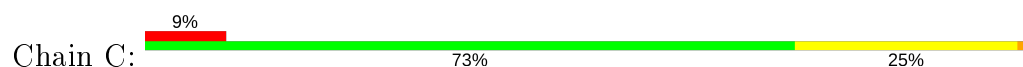
#### • Molecule 1: Purple acid phosphatase

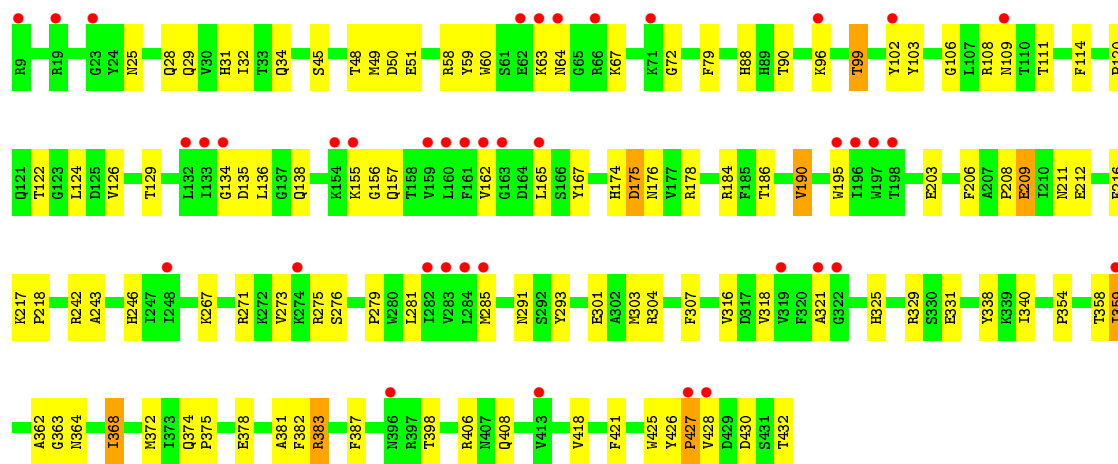


#### • Molecule 1: Purple acid phosphatase

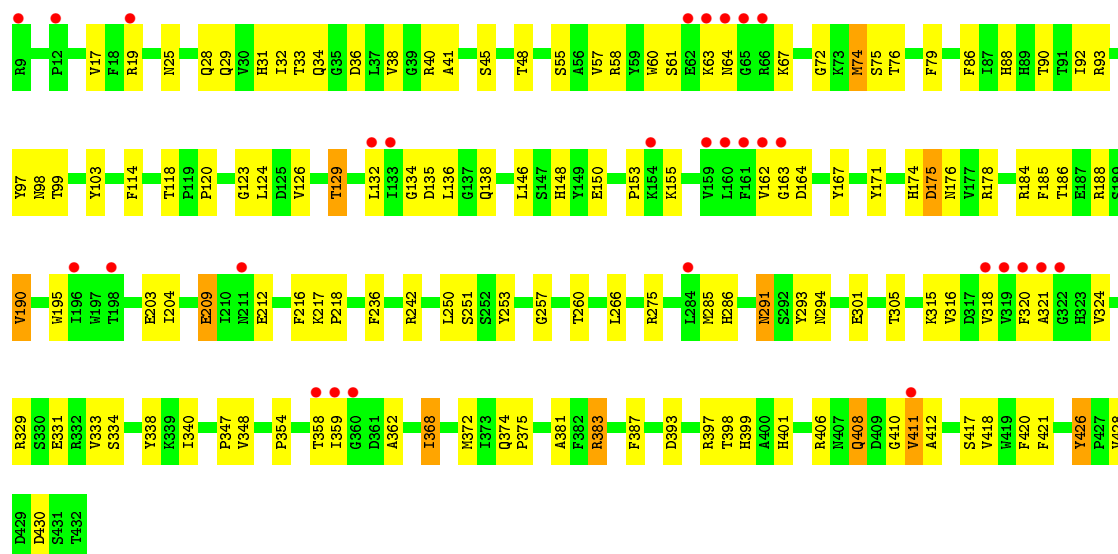


#### • Molecule 1: Purple acid phosphatase





• Molecule 1: Purple acid phosphatase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.72Å 188.47Å 192.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.00 – 2.20 33.33 – 2.20	Depositor EDS
% Data completeness (in resolution range)	86.9 (33.00-2.20) 86.7 (33.33-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.42 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.224 , 0.254 0.244 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.7	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 48.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.014 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	14782	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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: ZN, NAG, F, NA, SO4, FE

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	0.38	0/3606	0.61	0/4905
1	B	0.40	0/3606	0.61	0/4905
1	C	0.36	0/3606	0.56	0/4905
1	D	0.38	0/3606	0.58	0/4905
All	All	0.38	0/14424	0.59	0/19620

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	3487	0	3298	91	0
1	B	3487	0	3298	94	0
1	C	3487	0	3296	96	0
1	D	3487	0	3297	108	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	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	10	0	0	0	0
4	B	10	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	56	0	52	0	0
6	B	56	0	52	5	0
6	C	56	0	52	0	0
6	D	56	0	52	0	0
7	A	3	0	0	0	0
7	B	3	0	0	0	0
7	C	3	0	0	0	0
7	D	2	0	0	0	0
8	A	150	0	0	3	0
8	B	168	0	0	1	0
8	C	105	0	0	2	0
8	D	124	0	0	2	0
All	All	14782	0	13397	389	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 14.

All (389) 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:B:316:VAL:HG23	1:B:354:PRO:HB3	1.36	1.04
1:D:316:VAL:HG23	1:D:354:PRO:HB3	1.50	0.90
1:C:217:LYS:HB3	1:C:218:PRO:HD3	1.51	0.90
1:A:316:VAL:HG23	1:A:354:PRO:HB3	1.56	0.88
1:D:28:GLN:HE21	1:D:29:GLN:HE21	1.20	0.87
1:D:153:PRO:HG3	1:D:412:ALA:HB2	1.55	0.86
1:C:316:VAL:HG23	1:C:354:PRO:HB3	1.58	0.85
1:C:291:ASN:HD21	1:C:293:TYR:HB2	1.41	0.84
1:D:217:LYS:HB3	1:D:218:PRO:HD3	1.61	0.82
1:A:129:THR:HG22	1:A:393:ASP:OD1	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:ARG:HH12	1:B:94:LYS:HA	1.45	0.81
1:D:411:VAL:HG12	1:D:412:ALA:H	1.45	0.81
1:C:378:GLU:H	1:C:378:GLU:CD	1.83	0.80
1:A:217:LYS:HB3	1:A:218:PRO:HD3	1.63	0.80
1:B:17:VAL:HG21	1:B:185:PHE:HD1	1.47	0.79
1:A:368:ILE:HD12	1:A:385:ALA:HB1	1.66	0.77
1:B:217:LYS:HB3	1:B:218:PRO:HD3	1.68	0.75
1:B:316:VAL:HG23	1:B:354:PRO:CB	2.14	0.75
1:C:28:GLN:HE21	1:C:29:GLN:HE21	1.33	0.75
1:D:61:SER:HB3	1:D:64:ASN:HB3	1.69	0.75
1:D:74:MET:HE3	1:D:86:PHE:HD1	1.51	0.74
1:A:34:GLN:NE2	1:A:242:ARG:HE	1.86	0.73
1:C:63:LYS:HG3	1:C:64:ASN:H	1.54	0.73
1:D:34:GLN:NE2	1:D:242:ARG:HE	1.87	0.73
1:A:79:PHE:O	1:A:212:GLU:OE2	2.08	0.72
1:A:63:LYS:HG3	1:A:64:ASN:H	1.54	0.72
1:B:291:ASN:HD21	1:B:293:TYR:HB2	1.54	0.72
1:D:408:GLN:H	1:D:408:GLN:HE21	1.35	0.72
1:B:97:TYR:O	1:B:99:THR:HG22	1.89	0.71
1:D:162:VAL:HG21	1:D:321:ALA:HA	1.73	0.71
1:D:291:ASN:HD21	1:D:293:TYR:HB2	1.56	0.70
1:D:74:MET:HE1	1:D:76:THR:HG23	1.72	0.70
1:A:291:ASN:HD21	1:A:293:TYR:HB2	1.57	0.70
1:C:421:PHE:CD2	1:C:430:ASP:HB3	2.27	0.70
1:B:74:MET:HE1	1:B:76:THR:HG23	1.73	0.69
1:D:372:MET:SD	1:D:383:ARG:HD3	2.33	0.69
1:A:368:ILE:HD13	1:A:369:ASP:N	2.08	0.68
1:B:155:LYS:HD2	1:B:155:LYS:O	1.94	0.68
1:B:129:THR:HG22	1:B:157:GLN:HE21	1.58	0.67
1:D:316:VAL:HG23	1:D:354:PRO:CB	2.25	0.67
1:D:411:VAL:HG12	1:D:412:ALA:N	2.10	0.66
1:D:74:MET:HE1	1:D:75:SER:C	2.15	0.66
1:A:316:VAL:HG23	1:A:354:PRO:CB	2.24	0.66
1:B:28:GLN:NE2	1:B:184:ARG:HE	1.93	0.66
1:D:329:ARG:CZ	1:D:418:VAL:HG21	2.26	0.66
1:C:96:LYS:HB2	1:C:99:THR:HG21	1.78	0.65
1:B:33:THR:HG21	8:B:572:HOH:O	1.96	0.65
1:D:286:HIS:CE1	8:D:567:HOH:O	2.49	0.65
1:D:28:GLN:NE2	1:D:29:GLN:HE21	1.92	0.65
1:B:368:ILE:HD12	1:B:385:ALA:HB1	1.77	0.65
1:B:40:ARG:NH1	1:B:94:LYS:HA	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:GLN:NE2	1:B:178:ARG:HH11	1.96	0.64
1:D:331:GLU:HG2	1:D:381:ALA:HB2	1.78	0.64
1:D:398:THR:OG1	1:D:399:HIS:HD2	1.81	0.64
1:B:398:THR:OG1	1:B:399:HIS:HD2	1.81	0.64
1:B:147:SER:OG	6:B:438:NAG:H61	1.98	0.64
1:B:421:PHE:CD2	1:B:428:VAL:HG13	2.33	0.64
1:C:28:GLN:NE2	1:C:184:ARG:HE	1.96	0.63
1:C:316:VAL:O	1:C:354:PRO:HB3	1.98	0.63
1:C:316:VAL:HG23	1:C:354:PRO:CB	2.28	0.63
1:A:162:VAL:HG21	1:A:321:ALA:HA	1.81	0.63
1:B:129:THR:CG2	1:B:157:GLN:HE21	2.11	0.63
1:B:79:PHE:O	1:B:212:GLU:OE2	2.16	0.62
1:A:162:VAL:HG21	1:A:321:ALA:CA	2.29	0.62
1:B:17:VAL:HG21	1:B:185:PHE:CD1	2.33	0.62
1:D:79:PHE:O	1:D:212:GLU:OE2	2.16	0.62
1:D:33:THR:HG21	8:D:552:HOH:O	1.99	0.62
1:A:368:ILE:HD13	1:A:369:ASP:H	1.65	0.61
1:C:129:THR:H	1:C:157:GLN:HE21	1.46	0.61
1:C:60:TRP:HB3	1:C:67:LYS:HA	1.81	0.61
1:A:28:GLN:HE21	1:A:29:GLN:HE21	1.47	0.61
1:B:17:VAL:CG2	1:B:185:PHE:HD1	2.13	0.61
1:D:162:VAL:HG21	1:D:321:ALA:CA	2.30	0.61
1:A:275:ARG:NH2	1:A:315:LYS:O	2.30	0.61
1:A:271:ARG:HG3	1:A:271:ARG:HH11	1.66	0.60
1:C:359:ILE:N	1:C:359:ILE:HD13	2.16	0.60
1:B:267:LYS:HE2	1:B:271:ARG:NH2	2.15	0.60
1:D:74:MET:CE	1:D:76:THR:HG23	2.32	0.60
1:D:25:ASN:HD21	1:D:48:THR:HB	1.67	0.60
1:A:42:MET:HE1	1:A:194:PRO:HD3	1.82	0.60
1:C:79:PHE:O	1:C:212:GLU:OE2	2.19	0.60
1:A:316:VAL:O	1:A:354:PRO:HB3	2.02	0.59
1:C:358:THR:HG21	8:C:455:HOH:O	2.02	0.59
1:A:138:GLN:NE2	1:A:178:ARG:HH11	1.99	0.59
1:D:421:PHE:CD2	1:D:430:ASP:HB3	2.37	0.59
1:D:74:MET:HE1	1:D:75:SER:O	2.03	0.58
1:C:25:ASN:ND2	1:C:48:THR:HB	2.18	0.58
1:C:217:LYS:HB3	1:C:218:PRO:CD	2.31	0.58
1:C:25:ASN:ND2	1:C:51:GLU:H	2.02	0.58
1:B:174:HIS:O	1:B:175:ASP:C	2.42	0.58
1:D:17:VAL:HG21	1:D:185:PHE:HD1	1.68	0.58
1:A:359:ILE:HD13	1:A:359:ILE:N	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:LYS:HG3	1:D:64:ASN:H	1.69	0.58
1:D:97:TYR:O	1:D:99:THR:HG23	2.04	0.57
1:B:162:VAL:HG21	1:B:321:ALA:HA	1.86	0.57
1:D:401:HIS:HE2	1:D:417:SER:HG	1.50	0.57
1:A:138:GLN:HE21	1:A:178:ARG:HH11	1.53	0.57
1:B:72:GLY:HA3	1:B:90:THR:OG1	2.04	0.57
1:B:74:MET:CE	1:B:76:THR:HG23	2.33	0.57
1:A:135:ASP:HB3	1:A:167:TYR:OH	2.04	0.57
1:A:357:ILE:HG22	1:A:359:ILE:CD1	2.35	0.57
1:A:398:THR:OG1	1:A:399:HIS:HD2	1.88	0.57
1:C:34:GLN:NE2	1:C:242:ARG:HE	2.02	0.57
1:A:421:PHE:CD2	1:A:430:ASP:HB3	2.40	0.57
1:C:398:THR:HB	1:C:426:TYR:HB2	1.86	0.57
1:D:136:LEU:HA	1:D:362:ALA:HB3	1.87	0.57
1:A:132:LEU:HD11	1:A:320:PHE:CZ	2.40	0.56
1:A:372:MET:SD	1:A:383:ARG:HD3	2.45	0.56
1:D:153:PRO:HG3	1:D:412:ALA:CB	2.34	0.56
1:C:25:ASN:HD21	1:C:48:THR:HB	1.71	0.56
1:A:29:GLN:O	1:A:31:HIS:HD2	1.88	0.56
1:B:421:PHE:CD2	1:B:430:ASP:HB3	2.40	0.56
1:A:34:GLN:HE21	1:A:242:ARG:HE	1.51	0.56
1:C:267:LYS:HE2	1:C:271:ARG:HH22	1.71	0.56
1:D:138:GLN:NE2	1:D:178:ARG:HH11	2.02	0.56
1:D:38:VAL:HG23	1:D:40:ARG:HG2	1.87	0.56
1:C:275:ARG:NH1	1:C:281:LEU:HB2	2.21	0.55
1:A:25:ASN:ND2	1:A:51:GLU:H	2.05	0.55
1:B:372:MET:SD	1:B:383:ARG:HD3	2.47	0.55
1:B:34:GLN:NE2	1:B:242:ARG:HE	2.03	0.55
1:C:134:GLY:HA3	1:C:162:VAL:HG12	1.89	0.55
1:D:134:GLY:CA	1:D:162:VAL:HG12	2.37	0.55
1:D:25:ASN:ND2	1:D:48:THR:HB	2.21	0.55
1:B:135:ASP:HB3	1:B:167:TYR:OH	2.07	0.55
1:C:174:HIS:O	1:C:175:ASP:C	2.45	0.55
1:D:333:VAL:HG12	1:D:334:SER:N	2.22	0.55
1:B:122:THR:HA	1:B:243:ALA:O	2.06	0.55
1:C:129:THR:HG23	1:C:156:GLY:HA2	1.89	0.55
1:D:186:THR:O	1:D:190:VAL:HG23	2.06	0.55
1:A:124:LEU:HG	1:A:397:ARG:HD3	1.88	0.55
1:B:406:ARG:HB3	1:B:408:GLN:OE1	2.07	0.55
1:C:72:GLY:HA3	1:C:90:THR:OG1	2.07	0.54
1:D:72:GLY:HA3	1:D:90:THR:OG1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:ASN:ND2	1:C:293:TYR:H	2.05	0.54
1:D:74:MET:HE3	1:D:86:PHE:CD1	2.37	0.54
1:C:108:ARG:C	1:C:109:ASN:HD22	2.11	0.54
1:D:134:GLY:HA3	1:D:162:VAL:HG12	1.90	0.54
1:C:421:PHE:CD2	1:C:428:VAL:HG23	2.43	0.54
1:B:190:VAL:HG22	1:B:195:TRP:CE2	2.43	0.53
1:C:136:LEU:HA	1:C:362:ALA:HB3	1.89	0.53
1:C:186:THR:O	1:C:190:VAL:HG23	2.08	0.53
1:B:33:THR:HG23	1:B:195:TRP:O	2.08	0.53
1:C:129:THR:HG22	1:C:157:GLN:HE21	1.72	0.53
1:B:325:HIS:O	1:B:368:ILE:HD13	2.08	0.53
1:C:329:ARG:NE	1:C:418:VAL:HG21	2.23	0.53
1:C:426:TYR:N	1:C:427:PRO:HD3	2.22	0.53
1:D:174:HIS:O	1:D:175:ASP:C	2.47	0.53
1:C:406:ARG:HB3	1:C:408:GLN:OE1	2.09	0.53
1:A:291:ASN:ND2	1:A:293:TYR:H	2.06	0.53
1:C:109:ASN:HD22	1:C:109:ASN:N	2.06	0.53
1:D:146:LEU:O	1:D:150:GLU:HG3	2.08	0.53
1:C:303:MET:HE3	1:C:307:PHE:HD2	1.73	0.53
1:A:25:ASN:ND2	1:A:48:THR:HB	2.23	0.53
1:A:318:VAL:HG22	1:A:420:PHE:CE2	2.44	0.52
1:D:150:GLU:OE2	1:D:188:ARG:HD2	2.09	0.52
1:B:17:VAL:HG22	1:B:185:PHE:HA	1.92	0.52
1:B:28:GLN:HE22	1:B:184:ARG:HH21	1.57	0.52
1:B:329:ARG:NE	1:B:418:VAL:HG21	2.24	0.52
1:B:25:ASN:ND2	1:B:51:GLU:H	2.08	0.52
1:D:162:VAL:CG2	1:D:321:ALA:HA	2.40	0.52
1:A:165:LEU:N	1:A:165:LEU:HD12	2.25	0.52
1:D:60:TRP:HB3	1:D:67:LYS:HA	1.92	0.52
1:B:55:SER:OG	1:B:88:HIS:HD2	1.92	0.51
1:A:357:ILE:HG22	1:A:359:ILE:HD12	1.93	0.51
1:D:36:ASP:HB3	1:D:41:ALA:HB3	1.93	0.51
1:A:174:HIS:O	1:A:175:ASP:C	2.48	0.51
1:A:63:LYS:HE2	1:A:99:THR:HB	1.91	0.51
1:D:203:GLU:O	1:D:216:PHE:HA	2.10	0.51
1:D:333:VAL:HG13	1:D:348:VAL:O	2.10	0.51
1:A:120:PRO:HD3	8:A:582:HOH:O	2.10	0.51
1:B:330:SER:O	1:B:355:VAL:HG13	2.11	0.51
1:D:17:VAL:CG2	1:D:185:PHE:HD1	2.23	0.51
1:A:134:GLY:HA3	1:A:162:VAL:HG12	1.93	0.51
1:A:18:PHE:O	1:A:184:ARG:NH1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:PRO:HG2	1:A:105:VAL:HG12	1.92	0.51
1:A:389:HIS:HD2	8:A:458:HOH:O	1.93	0.50
1:C:129:THR:CG2	1:C:157:GLN:HG3	2.40	0.50
1:D:34:GLN:HE21	1:D:242:ARG:HH21	1.59	0.50
1:D:359:ILE:O	1:D:359:ILE:HG13	2.09	0.50
1:C:209:GLU:H	1:C:209:GLU:CD	2.14	0.50
1:C:338:TYR:CZ	1:C:340:ILE:HA	2.46	0.50
1:C:28:GLN:HE22	1:C:184:ARG:HE	1.60	0.50
1:C:329:ARG:HH21	1:C:432:THR:HG21	1.76	0.50
1:C:325:HIS:O	1:C:368:ILE:HD13	2.11	0.50
1:D:148:HIS:CE1	1:D:410:GLY:HA2	2.47	0.50
1:D:33:THR:HG23	1:D:195:TRP:O	2.12	0.50
1:D:132:LEU:HD11	1:D:320:PHE:CZ	2.47	0.49
1:D:368:ILE:HG12	1:D:387:PHE:CZ	2.47	0.49
1:B:74:MET:HE3	1:B:75:SER:O	2.13	0.49
1:A:162:VAL:CG2	1:A:321:ALA:HA	2.41	0.49
1:B:27:PRO:HG2	1:B:105:VAL:HG12	1.94	0.49
1:A:203:GLU:O	1:A:216:PHE:HA	2.13	0.49
1:B:109:ASN:HD22	6:B:440:NAG:C7	2.25	0.49
1:C:120:PRO:HG2	1:C:126:VAL:HG11	1.94	0.49
1:C:31:HIS:CE1	1:C:45:SER:HB2	2.48	0.49
1:C:162:VAL:HG21	1:C:321:ALA:HA	1.93	0.49
1:B:275:ARG:NH2	1:B:315:LYS:O	2.35	0.49
1:B:27:PRO:CG	1:B:105:VAL:HG12	2.43	0.49
1:B:108:ARG:CB	6:B:440:NAG:H62	2.43	0.49
1:C:374:GLN:HG3	1:C:375:PRO:HA	1.94	0.49
1:A:316:VAL:CG2	1:A:354:PRO:HG3	2.43	0.48
1:C:103:TYR:CZ	1:C:114:PHE:HB2	2.48	0.48
1:D:17:VAL:HG21	1:D:185:PHE:CD1	2.47	0.48
1:C:59:TYR:HA	1:C:102:TYR:O	2.14	0.48
1:D:338:TYR:CZ	1:D:340:ILE:HA	2.47	0.48
1:A:163:GLY:O	1:A:164:ASP:HB2	2.13	0.48
1:A:190:VAL:HG13	1:A:195:TRP:CD1	2.48	0.48
1:B:46:TRP:CE2	1:B:105:VAL:HG13	2.48	0.48
1:B:129:THR:HG22	1:B:157:GLN:NE2	2.24	0.48
1:B:33:THR:HG22	1:B:34:GLN:N	2.28	0.48
1:B:364:ASN:OD1	1:B:365:TYR:N	2.45	0.48
1:C:281:LEU:CD2	1:C:316:VAL:HG12	2.43	0.48
1:C:25:ASN:HD22	1:C:50:ASP:H	1.60	0.48
1:B:96:LYS:HB2	1:B:99:THR:HG21	1.96	0.48
1:C:359:ILE:HD13	1:C:359:ILE:H	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:VAL:HG13	1:D:195:TRP:CD1	2.48	0.48
1:B:129:THR:HB	1:B:393:ASP:OD1	2.14	0.48
1:B:25:ASN:HD21	1:B:51:GLU:H	1.61	0.48
1:B:132:LEU:HD13	1:B:320:PHE:CE1	2.48	0.47
1:C:124:LEU:HD13	1:C:276:SER:O	2.14	0.47
1:A:21:PRO:HG2	8:A:524:HOH:O	2.13	0.47
1:C:190:VAL:HG13	1:C:195:TRP:CG	2.49	0.47
1:C:203:GLU:O	1:C:216:PHE:HA	2.14	0.47
1:B:28:GLN:NE2	1:B:184:ARG:NE	2.62	0.47
1:B:74:MET:HE2	1:B:75:SER:CA	2.44	0.47
1:A:46:TRP:CE2	1:A:105:VAL:HG13	2.49	0.47
1:C:135:ASP:HB3	1:C:167:TYR:OH	2.15	0.47
1:C:32:ILE:HG12	1:C:190:VAL:O	2.14	0.47
1:C:45:SER:HA	1:C:88:HIS:O	2.14	0.47
1:D:34:GLN:HE22	1:D:242:ARG:HE	1.61	0.47
1:A:406:ARG:HB3	1:A:408:GLN:OE1	2.15	0.47
1:B:368:ILE:HD13	1:B:369:ASP:N	2.29	0.47
1:C:109:ASN:ND2	1:C:109:ASN:N	2.63	0.47
1:A:66:ARG:HH11	1:A:66:ARG:HG2	1.80	0.47
1:B:162:VAL:HG21	1:B:321:ALA:CA	2.44	0.47
1:C:285:MET:HE2	1:C:303:MET:HE1	1.97	0.47
1:D:204:ILE:HD11	1:D:253:TYR:CG	2.50	0.47
1:D:333:VAL:HG11	1:D:347:PRO:HB3	1.96	0.47
1:D:58:ARG:O	1:D:103:TYR:HA	2.15	0.47
1:A:129:THR:HG23	1:A:157:GLN:HE21	1.80	0.47
1:A:190:VAL:HG22	1:A:195:TRP:CE2	2.50	0.47
1:C:206:PHE:CZ	1:C:208:PRO:HG3	2.49	0.47
1:C:58:ARG:O	1:C:103:TYR:HA	2.14	0.46
1:A:27:PRO:CG	1:A:105:VAL:HG12	2.45	0.46
1:A:162:VAL:HG22	1:A:162:VAL:O	2.15	0.46
1:B:33:THR:HG22	1:B:34:GLN:H	1.81	0.46
1:D:411:VAL:CG1	1:D:412:ALA:H	2.13	0.46
1:A:374:GLN:HE21	1:A:375:PRO:HA	1.80	0.46
1:C:124:LEU:HD12	1:C:279:PRO:HD3	1.97	0.46
1:D:103:TYR:CE1	1:D:114:PHE:HB2	2.51	0.46
1:A:325:HIS:HA	1:A:360:GLY:O	2.16	0.46
1:D:135:ASP:HB3	1:D:167:TYR:OH	2.15	0.46
1:D:103:TYR:CZ	1:D:114:PHE:HB2	2.50	0.45
1:D:275:ARG:NH2	1:D:315:LYS:O	2.39	0.45
1:B:285:MET:O	1:B:321:ALA:HA	2.15	0.45
1:C:372:MET:SD	1:C:383:ARG:HD3	2.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:ASN:HD21	1:A:48:THR:HB	1.80	0.45
1:B:291:ASN:ND2	1:B:293:TYR:H	2.14	0.45
1:B:294:ASN:HD22	1:B:371:ASN:CG	2.19	0.45
1:D:217:LYS:HB3	1:D:218:PRO:CD	2.38	0.45
1:C:134:GLY:CA	1:C:162:VAL:HG12	2.46	0.45
1:A:25:ASN:HD21	1:A:51:GLU:H	1.64	0.45
1:A:55:SER:OG	1:A:88:HIS:HD2	2.00	0.45
1:D:406:ARG:HB3	1:D:408:GLN:NE2	2.31	0.45
1:A:184:ARG:HB2	1:A:184:ARG:HH11	1.82	0.45
1:B:129:THR:H	1:B:157:GLN:HE21	1.65	0.45
1:B:154:LYS:NZ	1:B:391:MET:HG3	2.32	0.45
1:B:74:MET:HE3	1:B:75:SER:C	2.38	0.45
1:A:60:TRP:HB3	1:A:67:LYS:HA	1.99	0.45
1:D:32:ILE:HG12	1:D:190:VAL:O	2.16	0.45
1:A:134:GLY:CA	1:A:162:VAL:HG12	2.47	0.45
1:A:72:GLY:HA3	1:A:90:THR:OG1	2.16	0.45
1:D:120:PRO:HG2	1:D:126:VAL:HG11	1.98	0.45
1:D:324:VAL:HB	1:D:358:THR:HG21	1.99	0.45
1:D:410:GLY:C	1:D:411:VAL:HG23	2.37	0.45
1:A:162:VAL:HG21	1:A:321:ALA:C	2.37	0.44
1:C:34:GLN:HE21	1:C:242:ARG:HE	1.65	0.44
1:C:368:ILE:HG12	1:C:387:PHE:CZ	2.52	0.44
1:C:425:TRP:C	1:C:427:PRO:HD3	2.36	0.44
1:D:333:VAL:HG11	1:D:347:PRO:CB	2.48	0.44
1:A:230:SER:O	1:A:231:GLN:HB2	2.18	0.44
1:A:66:ARG:NH1	1:A:68:ARG:HG2	2.32	0.44
1:B:109:ASN:ND2	6:B:440:NAG:C7	2.80	0.44
1:C:162:VAL:HG21	1:C:321:ALA:CA	2.47	0.44
1:B:25:ASN:ND2	1:B:48:THR:HB	2.32	0.44
1:D:74:MET:CE	1:D:75:SER:O	2.65	0.44
1:C:329:ARG:HH11	1:C:329:ARG:HB3	1.83	0.44
1:B:206:PHE:CZ	1:B:208:PRO:HG3	2.51	0.44
1:C:301:GLU:OE1	1:C:304:ARG:NH1	2.51	0.44
1:A:60:TRP:CE3	1:A:67:LYS:HG2	2.52	0.44
1:C:28:GLN:NE2	1:C:29:GLN:HE21	2.10	0.44
1:A:285:MET:O	1:A:321:ALA:HA	2.17	0.44
1:D:301:GLU:O	1:D:305:THR:HG23	2.17	0.44
1:D:55:SER:OG	1:D:88:HIS:HD2	2.01	0.44
1:B:134:GLY:CA	1:B:162:VAL:HG12	2.48	0.43
1:B:190:VAL:HG13	1:B:195:TRP:CG	2.53	0.43
1:C:363:GLY:O	1:C:364:ASN:C	2.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:257:GLY:O	1:D:260:THR:HG23	2.18	0.43
1:D:28:GLN:NE2	1:D:184:ARG:HE	2.16	0.43
1:B:162:VAL:O	1:B:162:VAL:HG22	2.18	0.43
1:C:122:THR:HA	1:C:243:ALA:O	2.18	0.43
1:B:187:GLU:O	1:B:189:SER:N	2.51	0.43
1:C:138:GLN:NE2	1:C:178:ARG:HH11	2.17	0.43
1:D:136:LEU:HA	1:D:362:ALA:CB	2.49	0.43
1:D:163:GLY:O	1:D:164:ASP:HB2	2.18	0.43
1:B:28:GLN:HG3	1:B:29:GLN:HG3	2.01	0.43
1:B:316:VAL:O	1:B:354:PRO:HB3	2.18	0.43
1:D:93:ARG:NH1	1:D:93:ARG:HB3	2.33	0.43
1:A:374:GLN:HG3	1:A:375:PRO:HA	2.00	0.43
1:C:106:GLY:O	1:C:111:THR:HG22	2.18	0.43
1:B:136:LEU:HA	1:B:362:ALA:HB3	2.01	0.43
1:B:391:MET:O	1:B:402:PHE:HA	2.19	0.43
1:D:19:ARG:HG2	1:D:19:ARG:HH11	1.84	0.43
1:D:190:VAL:HG13	1:D:195:TRP:CG	2.53	0.43
1:D:124:LEU:HD23	1:D:397:ARG:CZ	2.49	0.43
1:A:364:ASN:OD1	1:A:365:TYR:N	2.52	0.43
1:D:236:PHE:O	1:D:251:SER:HB2	2.19	0.43
1:C:331:GLU:HG2	1:C:381:ALA:HB2	2.01	0.42
1:C:329:ARG:CZ	1:C:418:VAL:HG21	2.49	0.42
1:D:57:VAL:HG11	1:D:92:ILE:HD11	2.00	0.42
1:B:318:VAL:HG22	1:B:420:PHE:CE2	2.55	0.42
1:A:186:THR:O	1:A:190:VAL:HG23	2.18	0.42
1:B:209:GLU:CD	1:B:209:GLU:H	2.21	0.42
1:D:318:VAL:HG22	1:D:420:PHE:CE2	2.55	0.42
1:D:61:SER:HB3	1:D:64:ASN:CB	2.42	0.42
1:A:56:ALA:HB1	1:A:69:ILE:HD11	2.01	0.42
1:A:74:MET:SD	1:A:75:SER:N	2.93	0.42
1:C:120:PRO:HD3	8:C:525:HOH:O	2.18	0.42
1:A:376:GLN:NE2	1:A:383:ARG:HG2	2.35	0.42
1:A:58:ARG:O	1:A:103:TYR:HA	2.19	0.42
1:B:186:THR:O	1:B:190:VAL:HG23	2.19	0.42
1:C:60:TRP:CE3	1:C:67:LYS:HG2	2.55	0.42
1:D:421:PHE:HB3	1:D:426:TYR:O	2.20	0.42
1:A:190:VAL:HG13	1:A:195:TRP:CG	2.55	0.42
1:C:165:LEU:N	1:C:165:LEU:HD12	2.35	0.42
1:C:329:ARG:HH12	1:C:382:PHE:CB	2.33	0.42
1:A:206:PHE:CZ	1:A:208:PRO:HG3	2.55	0.42
1:B:103:TYR:CZ	1:B:114:PHE:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:TYR:CE1	1:D:178:ARG:HG3	2.55	0.42
1:D:250:LEU:HD21	1:D:266:LEU:HD13	2.01	0.42
1:D:31:HIS:CE1	1:D:45:SER:HB2	2.55	0.42
1:A:208:PRO:HD2	1:A:209:GLU:OE2	2.20	0.41
1:D:285:MET:O	1:D:321:ALA:HA	2.19	0.41
1:B:165:LEU:HD12	1:B:165:LEU:N	2.35	0.41
1:B:16:ASP:O	1:B:19:ARG:HB2	2.20	0.41
1:C:329:ARG:NH1	1:C:329:ARG:HB3	2.36	0.41
1:A:59:TYR:HA	1:A:102:TYR:O	2.20	0.41
1:C:136:LEU:HA	1:C:362:ALA:CB	2.50	0.41
1:C:63:LYS:HG3	1:C:64:ASN:N	2.30	0.41
1:D:29:GLN:O	1:D:31:HIS:HD2	2.02	0.41
1:A:25:ASN:HD22	1:A:50:ASP:H	1.69	0.41
1:A:46:TRP:CG	1:A:105:VAL:HG11	2.56	0.41
1:A:132:LEU:HD13	1:A:320:PHE:CE1	2.55	0.41
1:A:41:ALA:O	1:A:42:MET:HG2	2.20	0.41
1:A:51:GLU:HB2	1:A:52:PRO:HD2	2.02	0.41
1:B:120:PRO:HG2	1:B:126:VAL:HG11	2.03	0.41
1:B:134:GLY:HA3	1:B:162:VAL:HG12	2.02	0.41
1:D:291:ASN:ND2	1:D:293:TYR:H	2.18	0.41
1:A:18:PHE:CD1	1:A:181:THR:HB	2.56	0.41
1:B:34:GLN:HE21	1:B:242:ARG:HE	1.66	0.41
1:C:267:LYS:HE2	1:C:271:ARG:NH2	2.35	0.41
1:D:98:ASN:HA	1:D:118:THR:O	2.21	0.41
1:A:426:TYR:N	1:A:427:PRO:HD3	2.35	0.41
1:B:58:ARG:O	1:B:103:TYR:HA	2.21	0.41
1:C:60:TRP:CD2	1:C:67:LYS:HG2	2.56	0.41
1:D:178:ARG:HA	1:D:178:ARG:HD3	1.96	0.41
1:D:316:VAL:HG23	1:D:354:PRO:CG	2.50	0.41
1:D:74:MET:CE	1:D:76:THR:CG2	2.98	0.41
1:A:338:TYR:CZ	1:A:340:ILE:HA	2.56	0.41
1:C:242:ARG:O	1:C:243:ALA:HB3	2.21	0.41
1:C:285:MET:O	1:C:321:ALA:HA	2.21	0.41
1:D:316:VAL:O	1:D:354:PRO:HB3	2.21	0.41
1:D:129:THR:HB	1:D:393:ASP:OD1	2.21	0.41
1:B:28:GLN:HE21	1:B:29:GLN:HE21	1.67	0.41
1:B:81:ASN:ND2	6:B:437:NAG:C7	2.83	0.41
1:C:246:HIS:CE1	1:C:273:VAL:HG22	2.56	0.41
1:A:236:PHE:O	1:A:251:SER:HB2	2.21	0.40
1:C:129:THR:HG22	1:C:157:GLN:HG3	2.02	0.40
1:A:246:HIS:HB2	1:A:278:THR:OG1	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:VAL:HG13	1:C:195:TRP:CD1	2.56	0.40
1:C:275:ARG:HH12	1:C:281:LEU:H	1.69	0.40
1:D:209:GLU:CD	1:D:209:GLU:H	2.23	0.40
1:B:138:GLN:HE21	1:B:178:ARG:HH11	1.67	0.40
1:C:303:MET:HE3	1:C:307:PHE:CD2	2.54	0.40
1:D:374:GLN:HG3	1:D:375:PRO:HA	2.03	0.40
1:B:31:HIS:CE1	1:B:45:SER:HB2	2.57	0.40
1:B:348:VAL:HG22	1:B:349:LYS:N	2.37	0.40
1:D:123:GLY:HA3	1:D:126:VAL:HG23	2.03	0.40
1:B:74:MET:HE2	1:B:75:SER:HA	2.03	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	422/424 (100%)	396 (94%)	24 (6%)	2 (0%)	29	31
1	B	422/424 (100%)	395 (94%)	25 (6%)	2 (0%)	29	31
1	C	422/424 (100%)	391 (93%)	28 (7%)	3 (1%)	22	22
1	D	422/424 (100%)	392 (93%)	27 (6%)	3 (1%)	22	22
All	All	1688/1696 (100%)	1574 (93%)	104 (6%)	10 (1%)	25	26

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	ASP
1	B	175	ASP
1	D	175	ASP
1	D	411	VAL
1	C	155	LYS

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Mol	Chain	Res	Type
1	C	175	ASP
1	A	65	GLY
1	B	188	ARG
1	D	155	LYS
1	C	427	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	372/373 (100%)	362 (97%)	10 (3%)	44	57
1	B	372/373 (100%)	357 (96%)	15 (4%)	31	40
1	C	372/373 (100%)	362 (97%)	10 (3%)	44	57
1	D	372/373 (100%)	360 (97%)	12 (3%)	39	50
All	All	1488/1492 (100%)	1441 (97%)	47 (3%)	39	50

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	64	ASN
1	A	99	THR
1	A	176	ASN
1	A	184	ARG
1	A	209	GLU
1	A	359	ILE
1	A	368	ILE
1	A	383	ARG
1	A	408	GLN
1	B	20	VAL
1	B	25	ASN
1	B	64	ASN
1	B	74	MET
1	B	99	THR
1	B	109	ASN

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Mol	Chain	Res	Type
1	B	129	THR
1	B	132	LEU
1	B	155	LYS
1	B	176	ASN
1	B	209	GLU
1	B	368	ILE
1	B	383	ARG
1	B	396	ASN
1	B	408	GLN
1	C	49	MET
1	C	99	THR
1	C	176	ASN
1	C	190	VAL
1	C	209	GLU
1	C	211	ASN
1	C	318	VAL
1	C	359	ILE
1	C	368	ILE
1	C	383	ARG
1	D	74	MET
1	D	129	THR
1	D	176	ASN
1	D	190	VAL
1	D	209	GLU
1	D	291	ASN
1	D	294	ASN
1	D	368	ILE
1	D	383	ARG
1	D	408	GLN
1	D	426	TYR
1	D	428	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	28	GLN
1	A	31	HIS
1	A	34	GLN
1	A	64	ASN
1	A	88	HIS
1	A	138	GLN

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Mol	Chain	Res	Type
1	A	157	GLN
1	A	291	ASN
1	A	371	ASN
1	A	374	GLN
1	A	376	GLN
1	A	389	HIS
1	A	399	HIS
1	A	424	HIS
1	B	25	ASN
1	B	28	GLN
1	B	34	GLN
1	B	64	ASN
1	B	88	HIS
1	B	138	GLN
1	B	157	GLN
1	B	211	ASN
1	B	291	ASN
1	B	294	ASN
1	B	376	GLN
1	B	399	HIS
1	B	424	HIS
1	C	25	ASN
1	C	28	GLN
1	C	34	GLN
1	C	64	ASN
1	C	88	HIS
1	C	138	GLN
1	C	157	GLN
1	C	173	ASN
1	C	211	ASN
1	C	246	HIS
1	C	291	ASN
1	C	399	HIS
1	C	401	HIS
1	D	25	ASN
1	D	28	GLN
1	D	31	HIS
1	D	34	GLN
1	D	88	HIS
1	D	138	GLN
1	D	173	ASN
1	D	193	GLN

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Mol	Chain	Res	Type
1	D	211	ASN
1	D	291	ASN
1	D	294	ASN
1	D	371	ASN
1	D	374	GLN
1	D	376	GLN
1	D	389	HIS
1	D	399	HIS
1	D	407	ASN
1	D	408	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 ⓘ

Of 47 ligands modelled in this entry, 23 are monoatomic - leaving 24 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	$\# Z  > 2$
6	NAG	A	438	1	14,14,15	0.51	0	17,19,21	0.68	1 (5%)
6	NAG	D	440	1	14,14,15	0.56	0	17,19,21	0.73	0
4	SO4	B	435	7	4,4,4	0.26	0	6,6,6	0.05	0
4	SO4	C	435	7	4,4,4	0.27	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SO4	A	441	7	4,4,4	0.26	0	6,6,6	0.06	0
4	SO4	B	441	7	4,4,4	0.27	0	6,6,6	0.05	0
6	NAG	A	437	1	14,14,15	0.56	0	17,19,21	0.73	1 (5%)
4	SO4	D	435	7	4,4,4	0.26	0	6,6,6	0.06	0
6	NAG	B	438	1	14,14,15	0.61	0	17,19,21	0.72	1 (5%)
6	NAG	B	440	1	14,14,15	0.58	0	17,19,21	0.65	0
6	NAG	C	439	1	14,14,15	0.67	0	17,19,21	0.69	1 (5%)
6	NAG	A	439	1	14,14,15	0.68	0	17,19,21	0.75	0
4	SO4	A	435	7	4,4,4	0.26	0	6,6,6	0.05	0
4	SO4	D	441	7	4,4,4	0.25	0	6,6,6	0.06	0
6	NAG	B	437	1	14,14,15	0.64	0	17,19,21	0.71	0
6	NAG	C	440	1	14,14,15	0.60	0	17,19,21	0.69	0
6	NAG	C	437	1	14,14,15	0.60	0	17,19,21	0.70	0
4	SO4	C	441	7	4,4,4	0.26	0	6,6,6	0.06	0
6	NAG	B	439	1	14,14,15	0.70	0	17,19,21	0.93	1 (5%)
6	NAG	D	437	1	14,14,15	0.62	0	17,19,21	0.76	0
6	NAG	A	440	1	14,14,15	0.56	0	17,19,21	0.69	0
6	NAG	D	439	1	14,14,15	0.71	1 (7%)	17,19,21	0.80	0
6	NAG	C	438	1	14,14,15	0.49	0	17,19,21	0.64	0
6	NAG	D	438	1	14,14,15	0.51	0	17,19,21	0.65	0

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
6	NAG	A	438	1	-	0/6/23/26	0/1/1/1
6	NAG	B	438	1	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	B	440	1	-	4/6/23/26	0/1/1/1
6	NAG	B	437	1	-	2/6/23/26	0/1/1/1
6	NAG	A	437	1	-	4/6/23/26	0/1/1/1
6	NAG	C	437	1	-	4/6/23/26	0/1/1/1
6	NAG	A	440	1	-	3/6/23/26	0/1/1/1
6	NAG	C	439	1	1/1/5/7	4/6/23/26	0/1/1/1
6	NAG	D	437	1	-	2/6/23/26	0/1/1/1
6	NAG	A	439	1	-	4/6/23/26	0/1/1/1
6	NAG	C	438	1	-	3/6/23/26	0/1/1/1
6	NAG	B	439	1	1/1/5/7	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	D	438	1	-	2/6/23/26	0/1/1/1
6	NAG	D	439	1	-	2/6/23/26	0/1/1/1
6	NAG	D	440	1	-	4/6/23/26	0/1/1/1
6	NAG	C	440	1	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	439	NAG	C1-C2	2.22	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	439	NAG	C2-N2-C7	-2.21	119.75	122.90
6	C	439	NAG	C2-N2-C7	-2.20	119.77	122.90
6	A	438	NAG	C2-N2-C7	-2.05	119.99	122.90
6	B	438	NAG	C2-N2-C7	-2.04	119.99	122.90
6	A	437	NAG	C2-N2-C7	-2.01	120.04	122.90

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	438	NAG	C1
6	C	439	NAG	C1
6	B	439	NAG	C1

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	440	NAG	C8-C7-N2-C2
6	D	440	NAG	O7-C7-N2-C2
6	C	439	NAG	C8-C7-N2-C2
6	C	439	NAG	O7-C7-N2-C2
6	A	437	NAG	C8-C7-N2-C2
6	A	437	NAG	O7-C7-N2-C2
6	C	440	NAG	C8-C7-N2-C2
6	C	440	NAG	O7-C7-N2-C2
6	C	438	NAG	C8-C7-N2-C2
6	C	438	NAG	O7-C7-N2-C2
6	A	440	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
6	A	440	NAG	O7-C7-N2-C2
6	C	437	NAG	C8-C7-N2-C2
6	B	437	NAG	C8-C7-N2-C2
6	C	440	NAG	O5-C5-C6-O6
6	C	437	NAG	O7-C7-N2-C2
6	C	440	NAG	C4-C5-C6-O6
6	C	439	NAG	O5-C5-C6-O6
6	B	437	NAG	O7-C7-N2-C2
6	D	437	NAG	C8-C7-N2-C2
6	B	439	NAG	O5-C5-C6-O6
6	C	437	NAG	O5-C5-C6-O6
6	D	438	NAG	C4-C5-C6-O6
6	B	438	NAG	O5-C5-C6-O6
6	A	437	NAG	O5-C5-C6-O6
6	B	439	NAG	C4-C5-C6-O6
6	A	439	NAG	C4-C5-C6-O6
6	D	437	NAG	O7-C7-N2-C2
6	B	440	NAG	C4-C5-C6-O6
6	D	438	NAG	O5-C5-C6-O6
6	B	440	NAG	C8-C7-N2-C2
6	A	439	NAG	O5-C5-C6-O6
6	C	437	NAG	C4-C5-C6-O6
6	A	439	NAG	C8-C7-N2-C2
6	B	440	NAG	O5-C5-C6-O6
6	C	438	NAG	C1-C2-N2-C7
6	A	437	NAG	C4-C5-C6-O6
6	A	440	NAG	O5-C5-C6-O6
6	D	440	NAG	C4-C5-C6-O6
6	C	439	NAG	C4-C5-C6-O6
6	B	440	NAG	O7-C7-N2-C2
6	B	438	NAG	C8-C7-N2-C2
6	A	439	NAG	O7-C7-N2-C2
6	D	439	NAG	C4-C5-C6-O6
6	D	439	NAG	O5-C5-C6-O6
6	B	438	NAG	C4-C5-C6-O6
6	B	438	NAG	O7-C7-N2-C2
6	D	440	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	438	NAG	1	0
6	B	440	NAG	3	0
6	B	437	NAG	1	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	424/424 (100%)	-0.05	26 (6%) 21 20	21, 32, 49, 79	0
1	B	424/424 (100%)	-0.04	21 (4%) 28 27	21, 31, 48, 73	0
1	C	424/424 (100%)	0.31	40 (9%) 8 7	25, 39, 61, 84	0
1	D	424/424 (100%)	0.11	29 (6%) 17 16	22, 35, 51, 81	0
All	All	1696/1696 (100%)	0.08	116 (6%) 17 16	21, 34, 55, 84	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	64	ASN	6.3
1	A	64	ASN	5.4
1	C	160	LEU	5.0
1	B	64	ASN	4.6
1	D	63	LYS	4.6
1	C	162	VAL	4.5
1	C	19	ARG	4.3
1	C	161	PHE	4.3
1	D	162	VAL	4.2
1	D	65	GLY	4.2
1	C	159	VAL	4.0
1	D	411	VAL	3.8
1	D	160	LEU	3.8
1	D	359	ILE	3.7
1	D	321	ALA	3.7
1	C	413	VAL	3.7
1	C	63	LYS	3.6
1	D	66	ARG	3.5
1	A	162	VAL	3.5
1	C	64	ASN	3.5
1	C	66	ARG	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	132	LEU	3.4
1	B	63	LYS	3.3
1	B	163	GLY	3.3
1	D	133	ILE	3.3
1	A	320	PHE	3.3
1	A	321	ALA	3.3
1	B	319	VAL	3.2
1	C	109	ASN	3.2
1	C	163	GLY	3.1
1	D	322	GLY	3.1
1	B	160	LEU	3.1
1	C	102	TYR	3.1
1	C	96	LYS	3.1
1	D	62	GLU	3.1
1	D	320	PHE	3.1
1	A	66	ARG	3.0
1	C	198	THR	3.0
1	B	134	GLY	3.0
1	D	12	PRO	3.0
1	C	274	LYS	3.0
1	B	162	VAL	3.0
1	C	321	ALA	3.0
1	C	9	ARG	3.0
1	C	359	ILE	2.9
1	C	62	GLU	2.9
1	D	161	PHE	2.9
1	A	161	PHE	2.9
1	D	196	ILE	2.8
1	B	320	PHE	2.8
1	C	427	PRO	2.8
1	D	159	VAL	2.8
1	B	65	GLY	2.8
1	B	357	ILE	2.8
1	C	396	ASN	2.8
1	D	284	LEU	2.8
1	C	283	VAL	2.7
1	B	133	ILE	2.7
1	C	134	GLY	2.7
1	A	283	VAL	2.7
1	D	132	LEU	2.7
1	D	319	VAL	2.7
1	A	69	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	196	ILE	2.7
1	B	161	PHE	2.7
1	D	198	THR	2.7
1	A	133	ILE	2.6
1	A	285	MET	2.6
1	B	66	ARG	2.6
1	C	282	ILE	2.6
1	B	165	LEU	2.5
1	D	163	GLY	2.5
1	D	9	ARG	2.5
1	D	360	GLY	2.5
1	D	154	LYS	2.5
1	A	65	GLY	2.4
1	C	285	MET	2.4
1	C	322	GLY	2.4
1	C	195	TRP	2.4
1	C	155	LYS	2.4
1	B	285	MET	2.4
1	B	359	ILE	2.4
1	C	71	LYS	2.4
1	C	284	LEU	2.4
1	C	154	LYS	2.3
1	C	133	ILE	2.3
1	C	428	VAL	2.3
1	A	196	ILE	2.3
1	A	284	LEU	2.3
1	C	319	VAL	2.3
1	C	165	LEU	2.3
1	A	318	VAL	2.3
1	B	321	ALA	2.3
1	A	431	SER	2.3
1	C	23	GLY	2.3
1	A	159	VAL	2.3
1	C	197	TRP	2.2
1	D	318	VAL	2.2
1	B	109	ASN	2.2
1	A	197	TRP	2.2
1	A	107	LEU	2.2
1	A	357	ILE	2.2
1	A	19	ARG	2.1
1	D	358	THR	2.1
1	B	318	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	160	LEU	2.1
1	A	198	THR	2.1
1	D	211	ASN	2.1
1	A	63	LYS	2.1
1	C	248	ILE	2.1
1	B	19	ARG	2.1
1	A	322	GLY	2.1
1	A	358	THR	2.0
1	D	19	ARG	2.0
1	A	319	VAL	2.0
1	B	198	THR	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 [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
6	NAG	D	440	14/15	0.45	0.43	77,79,80,80	0
7	NA	A	443	1/1	0.45	0.26	103,103,103,103	0
6	NAG	C	440	14/15	0.49	0.36	79,81,82,82	0
6	NAG	A	440	14/15	0.56	0.35	74,75,78,79	0
6	NAG	B	440	14/15	0.58	0.38	70,72,72,73	0
7	NA	C	444	1/1	0.68	0.28	106,106,106,106	0
7	NA	D	442	1/1	0.73	0.22	73,73,73,73	0
6	NAG	C	439	14/15	0.75	0.20	63,65,66,67	0
7	NA	B	443	1/1	0.75	0.13	81,81,81,81	0
7	NA	B	444	1/1	0.78	0.33	98,98,98,98	0
6	NAG	B	439	14/15	0.81	0.14	38,44,47,49	0
6	NAG	A	439	14/15	0.81	0.17	43,48,49,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	D	441	5/5	0.82	0.22	94,94,94,95	0
7	NA	A	444	1/1	0.82	0.31	68,68,68,68	0
6	NAG	C	438	14/15	0.84	0.22	55,57,62,62	0
6	NAG	D	437	14/15	0.84	0.19	57,59,60,61	0
4	SO4	A	441	5/5	0.86	0.23	94,94,95,95	0
6	NAG	D	439	14/15	0.87	0.16	41,48,50,50	0
6	NAG	D	438	14/15	0.87	0.21	44,50,52,55	0
6	NAG	A	437	14/15	0.88	0.14	55,58,60,61	0
6	NAG	B	437	14/15	0.89	0.14	53,54,56,57	0
7	NA	C	442	1/1	0.89	0.16	75,75,75,75	0
6	NAG	C	437	14/15	0.90	0.13	53,56,59,60	0
6	NAG	B	438	14/15	0.91	0.17	36,41,44,47	0
7	NA	D	443	1/1	0.91	0.45	95,95,95,95	0
4	SO4	D	435	5/5	0.92	0.17	93,94,94,95	0
6	NAG	A	438	14/15	0.93	0.10	36,37,40,42	0
4	SO4	C	441	5/5	0.94	0.10	87,88,88,88	0
4	SO4	C	435	5/5	0.94	0.16	87,87,87,87	0
4	SO4	A	435	5/5	0.94	0.15	82,82,82,82	0
4	SO4	B	441	5/5	0.95	0.10	87,87,87,88	0
4	SO4	B	435	5/5	0.95	0.17	92,92,92,93	0
7	NA	A	442	1/1	0.96	0.13	69,69,69,69	0
7	NA	C	443	1/1	0.96	0.46	89,89,89,89	0
5	F	A	436	1/1	0.96	0.12	40,40,40,40	0
7	NA	B	442	1/1	0.97	0.15	90,90,90,90	0
2	FE	C	433	1/1	0.98	0.05	51,51,51,51	0
5	F	B	436	1/1	0.99	0.06	38,38,38,38	0
5	F	D	436	1/1	0.99	0.07	39,39,39,39	0
5	F	C	436	1/1	0.99	0.10	38,38,38,38	0
3	ZN	D	434	1/1	0.99	0.09	33,33,33,33	0
2	FE	A	433	1/1	0.99	0.05	47,47,47,47	0
2	FE	D	433	1/1	0.99	0.04	50,50,50,50	0
2	FE	B	433	1/1	1.00	0.03	46,46,46,46	0
3	ZN	B	434	1/1	1.00	0.08	34,34,34,34	0
3	ZN	C	434	1/1	1.00	0.08	33,33,33,33	0
3	ZN	A	434	1/1	1.00	0.09	32,32,32,32	0

## 6.5 Other polymers

There are no such residues in this entry.