



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:32 am GMT

PDB ID : 2D2I  
Title : Crystal Structure of NADP-Dependent Glyceraldehyde-3-Phosphate Dehydrogenase from *Synechococcus* Sp. complexed with Nadp+  
Authors : Kitatani, T.; Nakamura, Y.; Wada, K.; Kinoshita, T.; Tamoi, M.; Shigeoka, S.; Tada, T.  
Deposited on : 2005-09-09  
Resolution : 2.50 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : recalc28949

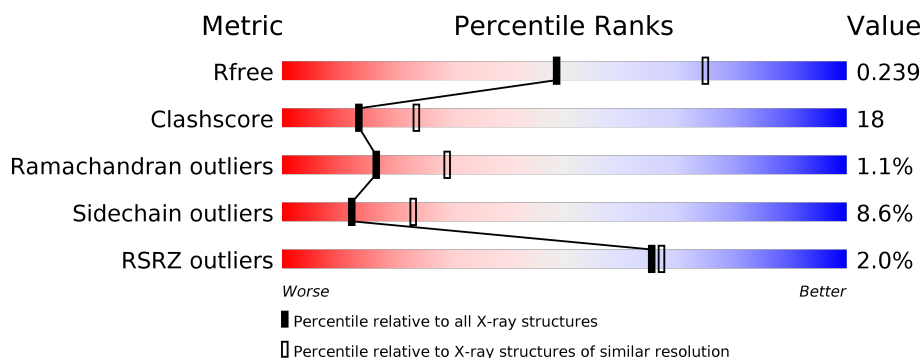
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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. 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	380	<div> <div>2%</div> <div>61% 24% 11%</div> </div>
1	B	380	<div> <div>2%</div> <div>63% 21% 5% 11%</div> </div>
1	O	380	<div> <div>2%</div> <div>62% 23% 11%</div> </div>
1	P	380	<div> <div>2%</div> <div>58% 28% 11%</div> </div>
1	Q	380	<div> <div>4%</div> <div>59% 27% 11%</div> </div>
1	R	380	<div> <div>2%</div> <div>61% 24% 11%</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
2	SO4	B	2339	-	-	-	X
2	SO4	O	3339	-	-	-	X
2	SO4	P	4339	-	-	-	X

## 2 Entry composition [i](#)

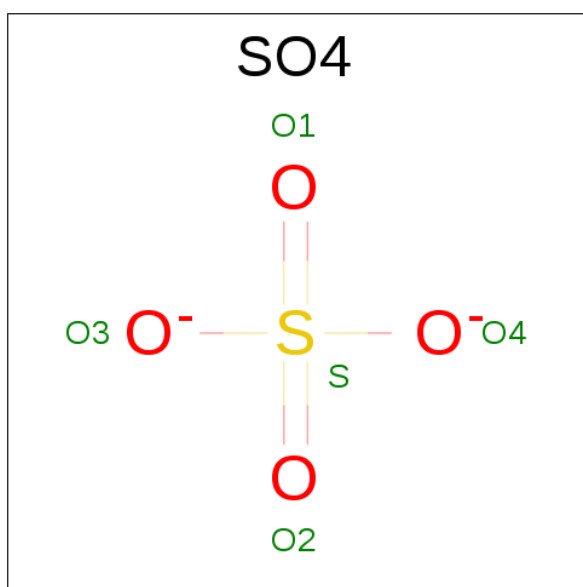
There are 4 unique types of molecules in this entry. The entry contains 16415 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 glyceraldehyde 3-phosphate dehydrogenase.

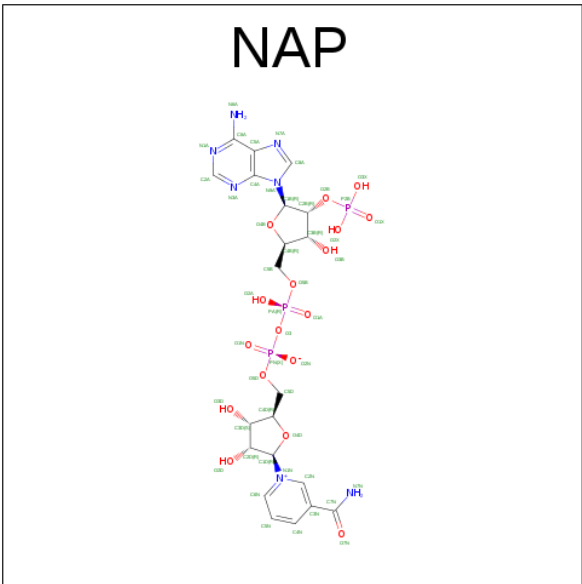
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2588	1625	454	500	9			
1	B	338	Total	C	N	O	S	0	0	0
			2588	1625	454	500	9			
1	O	338	Total	C	N	O	S	0	0	0
			2588	1625	454	500	9			
1	P	338	Total	C	N	O	S	0	0	0
			2588	1625	454	500	9			
1	Q	338	Total	C	N	O	S	0	0	0
			2588	1625	454	500	9			
1	R	338	Total	C	N	O	S	0	0	0
			2588	1625	454	500	9			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	O	1	Total O S 5 4 1	0	0
2	O	1	Total O S 5 4 1	0	0
2	P	1	Total O S 5 4 1	0	0
2	P	1	Total O S 5 4 1	0	0
2	Q	1	Total O S 5 4 1	0	0
2	Q	1	Total O S 5 4 1	0	0
2	R	1	Total O S 5 4 1	0	0
2	R	1	Total O S 5 4 1	0	0

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	B	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	O	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	P	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	Q	1	Total 48	C 21	N 7	O 17	P 3	0	0
3	R	1	Total 48	C 21	N 7	O 17	P 3	0	0

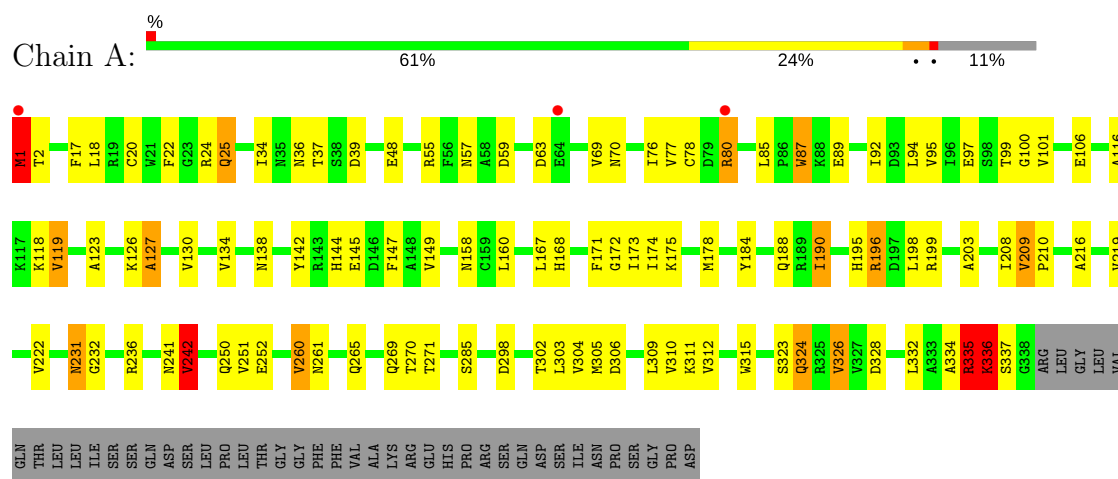
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	107	Total 107	O 107	0	0
4	B	142	Total 142	O 142	0	0
4	O	86	Total 86	O 86	0	0
4	P	82	Total 82	O 82	0	0
4	Q	47	Total 47	O 47	0	0
4	R	75	Total 75	O 75	0	0

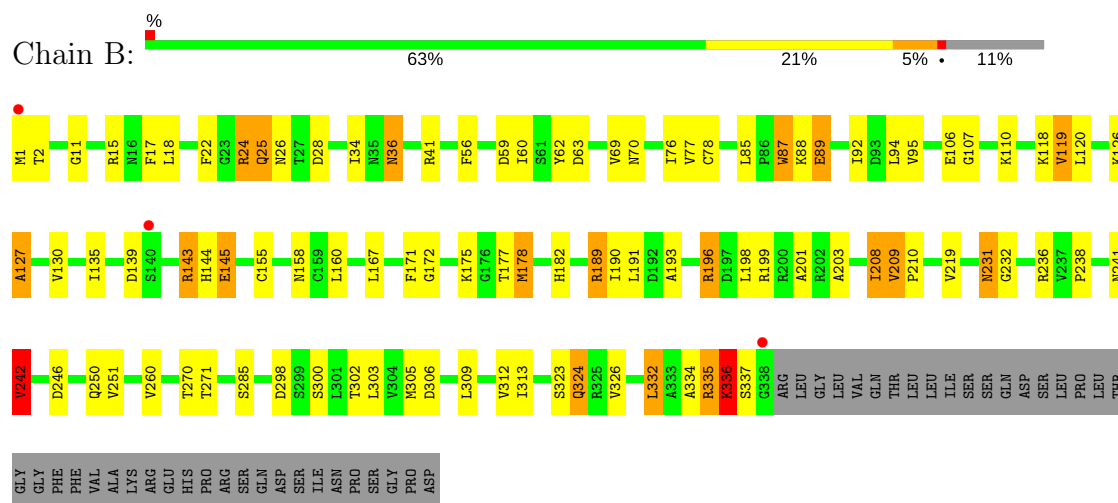
### 3 Residue-property plots

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

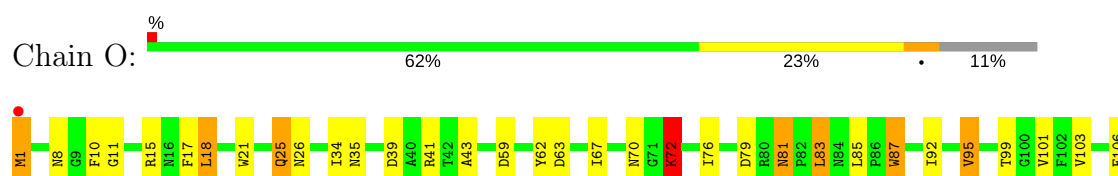
- Molecule 1: glyceraldehyde 3-phosphate dehydrogenase

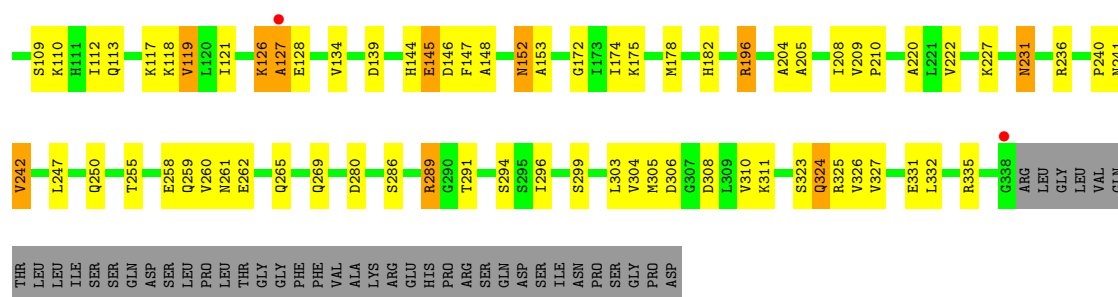


- Molecule 1: glyceraldehyde 3-phosphate dehydrogenase

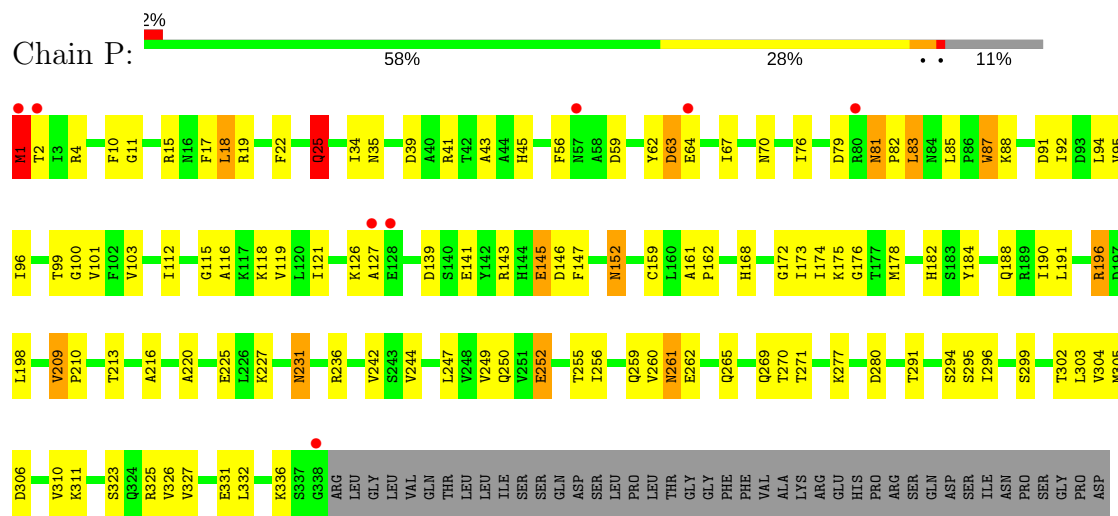


- Molecule 1: glyceraldehyde 3-phosphate dehydrogenase

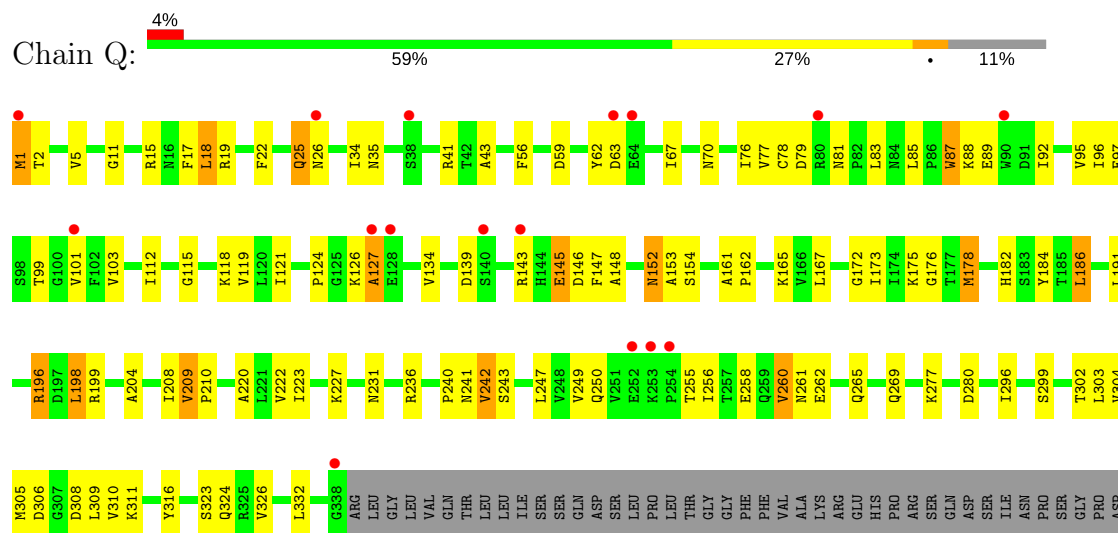




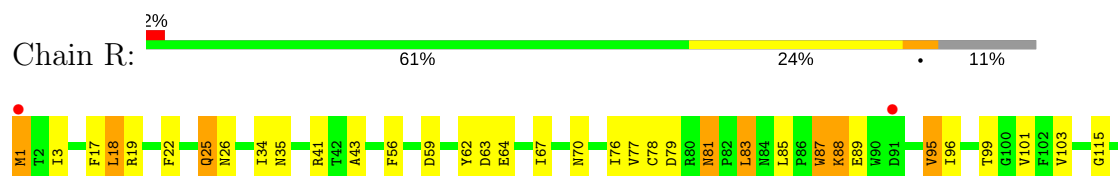
- Molecule 1: glyceraldehyde 3-phosphate dehydrogenase



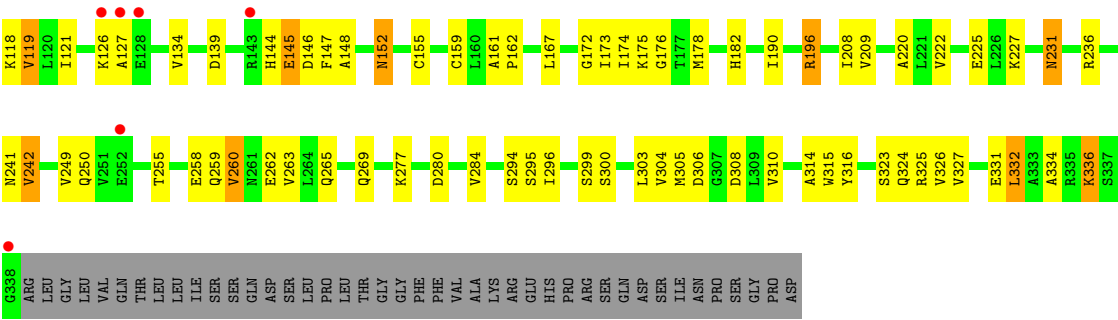
- Molecule 1: glyceraldehyde 3-phosphate dehydrogenase



- Molecule 1: glyceraldehyde 3-phosphate dehydrogenase







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	150.01Å 79.59Å 206.16Å 90.00° 101.31° 90.00°	Depositor
Resolution (Å)	19.96 – 2.50 19.95 – 2.50	Depositor EDS
% Data completeness (in resolution range)	85.9 (19.96-2.50) 86.0 (19.95-2.50)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.85 (at 2.50Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.191 , 0.240 0.190 , 0.239	Depositor DCC
$R_{free}$ test set	7199 reflections (10.13%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.3	Xtriage
Anisotropy	0.536	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 54.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	16415	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAP, SO4

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	0.61	0/2629	0.87	4/3575 (0.1%)
1	B	0.63	0/2629	0.88	1/3575 (0.0%)
1	O	0.61	0/2629	0.81	3/3575 (0.1%)
1	P	0.73	7/2629 (0.3%)	0.80	2/3575 (0.1%)
1	Q	0.50	0/2629	0.72	1/3575 (0.0%)
1	R	0.60	5/2629 (0.2%)	0.75	1/3575 (0.0%)
All	All	0.62	12/15774 (0.1%)	0.81	12/21450 (0.1%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	P	25	GLN	C-O	11.80	1.45	1.23
1	P	25	GLN	CB-CG	9.79	1.78	1.52
1	R	89	GLU	CB-CG	-8.74	1.35	1.52
1	R	89	GLU	CG-CD	-7.77	1.40	1.51
1	P	25	GLN	CA-CB	-7.67	1.37	1.53
1	P	252	GLU	CG-CD	-7.01	1.41	1.51
1	P	262	GLU	CB-CG	-6.91	1.39	1.52
1	R	89	GLU	CD-OE2	-5.85	1.19	1.25
1	P	1	MET	CG-SD	-5.66	1.66	1.81
1	R	88	LYS	CE-NZ	-5.61	1.35	1.49
1	P	252	GLU	CD-OE2	-5.56	1.19	1.25
1	R	1	MET	SD-CE	-5.21	1.48	1.77

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	25	GLN	CB-CA-C	-8.27	93.85	110.40
1	A	208	ILE	N-CA-C	-7.20	91.56	111.00
1	A	335	ARG	NE-CZ-NH1	-6.65	116.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	335	ARG	NE-CZ-NH2	6.62	123.61	120.30
1	B	208	ILE	N-CA-C	-6.50	93.44	111.00
1	P	25	GLN	N-CA-CB	-6.37	99.14	110.60
1	O	289	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	O	208	ILE	N-CA-C	-5.92	95.02	111.00
1	R	208	ILE	N-CA-C	-5.71	95.59	111.00
1	A	1	MET	CA-CB-CG	5.66	122.91	113.30
1	Q	208	ILE	N-CA-C	-5.53	96.08	111.00
1	O	72	LYS	CD-CE-NZ	5.30	123.88	111.70

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-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 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	2588	0	2615	114	0
1	B	2588	0	2615	97	0
1	O	2588	0	2615	83	0
1	P	2588	0	2615	121	0
1	Q	2588	0	2615	102	0
1	R	2588	0	2615	84	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	O	10	0	0	0	0
2	P	10	0	0	1	0
2	Q	10	0	0	0	0
2	R	10	0	0	0	0
3	A	48	0	25	2	0
3	B	48	0	25	0	0
3	O	48	0	25	0	0
3	P	48	0	25	3	0
3	Q	48	0	25	1	0
3	R	48	0	25	0	0
4	A	107	0	0	13	0
4	B	142	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	O	86	0	0	5	0
4	P	82	0	0	5	0
4	Q	47	0	0	3	0
4	R	75	0	0	2	0
All	All	16415	0	15840	568	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 18.

All (568) 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:P:25:GLN:CG	1:P:25:GLN:CB	1.79	1.61
1:A:324:GLN:HE21	1:A:324:GLN:HA	1.11	1.14
1:P:25:GLN:H	1:P:25:GLN:HG3	1.14	1.08
1:O:1:MET:O	1:O:1:MET:HE2	1.52	1.08
1:A:80:ARG:HG2	1:A:80:ARG:HH11	1.13	1.07
1:O:1:MET:HA	1:O:1:MET:HE3	1.42	1.01
1:A:160:LEU:HD22	1:A:178:MET:HE3	1.43	1.00
1:B:189:ARG:HG2	1:B:193:ALA:HB3	1.44	0.99
1:Q:196:ARG:NE	1:Q:196:ARG:H	1.61	0.98
1:B:160:LEU:HD22	1:B:178:MET:HE2	1.43	0.98
1:P:196:ARG:HE	1:P:196:ARG:H	1.02	0.98
1:Q:196:ARG:N	1:Q:196:ARG:HE	1.62	0.97
1:R:196:ARG:N	1:R:196:ARG:HE	1.63	0.96
1:R:196:ARG:H	1:R:196:ARG:NE	1.61	0.96
1:B:324:GLN:HE21	1:B:324:GLN:HA	1.27	0.95
1:Q:196:ARG:H	1:Q:196:ARG:HE	0.95	0.95
1:Q:1:MET:N	1:Q:1:MET:HE2	1.80	0.94
1:P:25:GLN:H	1:P:25:GLN:CG	1.81	0.94
1:O:196:ARG:H	1:O:196:ARG:HE	1.04	0.93
1:O:196:ARG:NE	1:O:196:ARG:H	1.68	0.92
1:O:196:ARG:HE	1:O:196:ARG:N	1.66	0.92
1:A:231:ASN:C	1:A:231:ASN:HD22	1.73	0.92
1:Q:1:MET:H3	1:Q:1:MET:HE2	1.31	0.90
1:O:304:VAL:HG22	1:O:310:VAL:HG12	1.52	0.90
1:Q:175:LYS:HD3	1:R:306:ASP:HB3	1.54	0.89
1:R:196:ARG:H	1:R:196:ARG:HE	0.91	0.88
1:B:209:VAL:HG22	1:B:236:ARG:HB2	1.55	0.87
1:B:231:ASN:HD22	1:B:232:GLY:H	1.21	0.87
1:P:1:MET:HE2	1:P:1:MET:N	1.89	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:196:ARG:N	1:P:196:ARG:HE	1.71	0.87
1:P:196:ARG:NE	1:P:196:ARG:H	1.73	0.86
1:O:1:MET:HA	1:O:1:MET:CE	2.06	0.86
1:P:25:GLN:CG	1:P:25:GLN:N	2.39	0.85
1:A:196:ARG:NE	1:A:196:ARG:H	1.74	0.85
1:A:231:ASN:OD1	1:B:303:LEU:HD21	1.77	0.85
1:Q:304:VAL:HG22	1:Q:310:VAL:HG12	1.58	0.84
1:A:324:GLN:NE2	1:A:324:GLN:HA	1.94	0.83
1:R:118:LYS:HE3	1:R:147:PHE:O	1.78	0.82
1:A:80:ARG:NH1	1:A:80:ARG:HG2	1.78	0.82
1:O:175:LYS:HE2	1:O:250:GLN:NE2	1.95	0.81
1:O:1:MET:CE	1:O:1:MET:CA	2.58	0.81
1:P:25:GLN:HG3	1:P:25:GLN:N	1.94	0.80
1:B:196:ARG:NE	1:B:196:ARG:H	1.80	0.80
1:P:331:GLU:HG3	4:P:6865:HOH:O	1.82	0.79
1:A:1:MET:HG2	1:A:2:THR:H	1.47	0.79
1:B:196:ARG:CD	1:B:196:ARG:H	1.96	0.79
1:A:59:ASP:H	1:A:70:ASN:ND2	1.82	0.78
1:O:1:MET:C	1:O:1:MET:HE2	2.03	0.77
1:B:231:ASN:HD22	1:B:232:GLY:N	1.80	0.77
1:Q:25:GLN:HE21	1:Q:26:ASN:H	1.33	0.77
1:A:1:MET:HE2	1:A:2:THR:N	1.99	0.77
1:P:25:GLN:CG	1:P:25:GLN:CA	2.63	0.76
1:Q:148:ALA:HA	4:Q:6627:HOH:O	1.85	0.76
1:P:118:LYS:HE3	1:P:147:PHE:O	1.87	0.75
1:B:25:GLN:HG2	1:B:26:ASN:H	1.52	0.75
1:A:175:LYS:HE2	1:B:306:ASP:HB3	1.68	0.74
1:Q:175:LYS:HE2	1:Q:250:GLN:NE2	2.03	0.73
1:Q:67:ILE:HD12	1:Q:76:ILE:HD11	1.69	0.73
1:R:304:VAL:HG22	1:R:310:VAL:HG12	1.70	0.73
1:A:196:ARG:HE	1:A:196:ARG:H	1.36	0.73
1:Q:209:VAL:HG22	1:Q:236:ARG:HB2	1.70	0.72
1:R:303:LEU:HD11	1:R:305:MET:HG2	1.71	0.72
1:A:231:ASN:HB2	4:A:6611:HOH:O	1.88	0.72
1:O:128:GLU:HG2	4:O:6461:HOH:O	1.89	0.71
1:O:59:ASP:H	1:O:70:ASN:HD21	1.36	0.71
1:A:323:SER:HA	1:A:326:VAL:HG13	1.72	0.71
1:R:182:HIS:HB3	1:R:236:ARG:HD3	1.72	0.71
1:O:41:ARG:HG3	1:O:62:TYR:OH	1.90	0.71
1:O:59:ASP:H	1:O:70:ASN:ND2	1.86	0.71
1:B:143:ARG:HD2	1:B:145:GLU:OE2	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:1:MET:C	1:Q:1:MET:HE3	2.12	0.70
1:A:306:ASP:HB3	1:B:175:LYS:HE2	1.74	0.70
1:B:59:ASP:H	1:B:70:ASN:ND2	1.91	0.69
1:B:171:PHE:HB3	1:B:251:VAL:CG1	2.22	0.69
1:B:171:PHE:HB3	1:B:251:VAL:HG11	1.75	0.69
1:A:324:GLN:HE21	1:A:324:GLN:CA	1.97	0.69
1:O:118:LYS:HE3	1:O:147:PHE:O	1.92	0.69
1:Q:43:ALA:HB3	1:Q:67:ILE:HD11	1.75	0.69
1:A:209:VAL:HG22	1:A:236:ARG:HB2	1.74	0.68
1:P:304:VAL:HG22	1:P:310:VAL:HG12	1.73	0.68
1:B:231:ASN:ND2	1:B:232:GLY:H	1.91	0.67
1:A:196:ARG:HD3	4:A:6769:HOH:O	1.94	0.67
1:R:78:CYS:SG	1:R:78:CYS:O	2.52	0.67
1:B:85:LEU:HD13	1:B:87:TRP:CZ2	2.30	0.66
1:P:99:THR:OG1	1:P:101:VAL:HG12	1.96	0.65
1:Q:25:GLN:NE2	1:Q:26:ASN:H	1.94	0.65
1:O:182:HIS:HB3	1:O:236:ARG:HD3	1.78	0.65
1:B:260:VAL:CG2	1:B:302:THR:HG21	2.27	0.65
1:P:182:HIS:HB3	1:P:236:ARG:HD3	1.76	0.65
1:P:209:VAL:HG22	1:P:236:ARG:HB2	1.78	0.65
1:P:1:MET:HE2	1:P:1:MET:H3	1.62	0.65
1:A:171:PHE:HB3	1:A:251:VAL:CG1	2.27	0.64
1:A:231:ASN:C	1:A:231:ASN:ND2	2.49	0.64
1:R:41:ARG:HG3	1:R:62:TYR:OH	1.98	0.64
1:P:25:GLN:CB	1:P:25:GLN:CD	2.62	0.64
1:A:171:PHE:HB3	1:A:251:VAL:HG11	1.81	0.63
1:P:141:GLU:HG3	4:P:6869:HOH:O	1.99	0.63
1:P:1:MET:HE3	1:P:1:MET:C	2.19	0.63
1:B:324:GLN:NE2	1:B:324:GLN:HA	2.08	0.63
1:Q:99:THR:OG1	1:Q:101:VAL:HG12	1.99	0.63
1:Q:41:ARG:HG3	1:Q:62:TYR:OH	1.99	0.63
1:A:59:ASP:H	1:A:70:ASN:HD21	1.45	0.62
1:A:24:ARG:HH12	1:A:324:GLN:NE2	1.98	0.62
1:P:175:LYS:CE	1:P:250:GLN:NE2	2.62	0.62
1:P:175:LYS:HE3	1:P:250:GLN:NE2	2.14	0.62
1:A:144:HIS:CD2	1:A:337:SER:HA	2.34	0.62
1:B:160:LEU:HD22	1:B:178:MET:CE	2.25	0.62
1:O:67:ILE:HD12	1:O:76:ILE:HD11	1.81	0.62
1:Q:41:ARG:HG3	1:Q:62:TYR:CZ	2.35	0.62
1:A:142:TYR:HD2	1:A:336:LYS:HD2	1.65	0.61
1:Q:306:ASP:HB3	1:R:175:LYS:HD3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:85:LEU:HD13	1:Q:87:TRP:CZ2	2.34	0.61
1:Q:303:LEU:HD11	1:Q:305:MET:HG2	1.81	0.61
1:A:126:LYS:HD2	4:A:6787:HOH:O	2.01	0.61
1:R:323:SER:HA	1:R:326:VAL:HG13	1.83	0.61
1:Q:210:PRO:HG2	1:R:315:TRP:HZ2	1.65	0.60
1:O:112:ILE:CD1	1:O:148:ALA:HB1	2.31	0.60
1:P:1:MET:HE2	1:P:1:MET:H2	1.66	0.60
1:P:25:GLN:HB2	1:P:25:GLN:HE21	1.64	0.60
1:P:87:TRP:CE3	1:P:92:ILE:HG13	2.36	0.60
1:B:189:ARG:CG	1:B:193:ALA:HB3	2.26	0.60
1:O:126:LYS:O	1:O:127:ALA:HB3	2.01	0.60
1:A:160:LEU:HD22	1:A:178:MET:CE	2.25	0.60
1:A:196:ARG:HE	1:A:196:ARG:N	1.99	0.60
1:A:306:ASP:HB3	1:B:175:LYS:CE	2.31	0.60
1:B:59:ASP:H	1:B:70:ASN:HD21	1.49	0.59
1:A:80:ARG:CG	1:A:80:ARG:HH11	1.97	0.59
1:P:174:ILE:HD12	1:P:250:GLN:HG2	1.83	0.59
1:R:103:VAL:HG23	1:R:126:LYS:HB2	1.83	0.59
1:O:1:MET:CA	1:O:1:MET:HE2	2.31	0.59
1:P:41:ARG:HG3	1:P:62:TYR:OH	2.02	0.59
1:P:59:ASP:H	1:P:70:ASN:ND2	2.00	0.59
1:R:59:ASP:H	1:R:70:ASN:ND2	2.01	0.59
1:P:327:VAL:O	1:P:331:GLU:HB2	2.02	0.59
1:A:196:ARG:CD	1:A:196:ARG:H	2.14	0.59
1:A:87:TRP:CE3	1:A:92:ILE:HG13	2.37	0.59
1:Q:182:HIS:HB3	1:Q:236:ARG:HD3	1.83	0.59
1:O:43:ALA:HB3	1:O:67:ILE:HD11	1.85	0.58
1:Q:324:GLN:OE1	1:Q:324:GLN:HA	2.03	0.58
1:R:303:LEU:CD1	1:R:305:MET:HG2	2.34	0.58
1:P:190:ILE:HD11	1:Q:204:ALA:HB3	1.86	0.58
1:A:1:MET:C	1:A:1:MET:HE2	2.23	0.58
1:Q:265:GLN:O	1:Q:269:GLN:HG3	2.03	0.58
1:A:199:ARG:NH2	1:B:298:ASP:OD1	2.37	0.58
1:A:309:LEU:HD13	1:A:309:LEU:C	2.23	0.58
1:P:1:MET:CE	1:P:1:MET:N	2.66	0.57
1:Q:152:ASN:OD1	1:Q:326:VAL:HA	2.03	0.57
1:A:285:SER:HB3	1:B:208:ILE:HB	1.86	0.57
1:P:216:ALA:HB3	4:P:6866:HOH:O	2.03	0.57
1:R:126:LYS:O	1:R:127:ALA:HB3	2.03	0.57
1:Q:308:ASP:OD2	1:R:175:LYS:NZ	2.36	0.57
1:R:99:THR:OG1	1:R:101:VAL:HG12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:126:LYS:O	1:Q:127:ALA:HB3	2.04	0.57
1:O:41:ARG:HG3	1:O:62:TYR:CZ	2.39	0.57
1:A:195:HIS:CE1	1:A:196:ARG:HD2	2.40	0.57
1:O:306:ASP:HB3	1:P:175:LYS:HD3	1.87	0.56
1:R:81:ASN:HD21	1:R:83:LEU:CD2	2.18	0.56
1:A:178:MET:O	1:A:232:GLY:HA3	2.04	0.56
1:B:88:LYS:HB3	1:B:89:GLU:OE1	2.06	0.56
1:Q:143:ARG:HB2	1:Q:146:ASP:OD2	2.05	0.56
1:Q:258:GLU:O	1:Q:262:GLU:HG3	2.05	0.56
1:O:145:GLU:H	1:O:145:GLU:CD	2.06	0.56
1:R:145:GLU:CD	1:R:145:GLU:H	2.08	0.56
1:A:1:MET:CE	1:A:2:THR:N	2.69	0.56
1:B:1:MET:HE2	1:B:2:THR:H	1.70	0.56
1:A:126:LYS:O	1:A:127:ALA:HB3	2.06	0.56
1:Q:303:LEU:CD1	1:Q:305:MET:HG2	2.35	0.56
1:B:24:ARG:HH21	1:B:24:ARG:CG	2.18	0.56
1:P:59:ASP:H	1:P:70:ASN:HD21	1.52	0.56
1:Q:59:ASP:H	1:Q:70:ASN:ND2	2.04	0.56
1:P:126:LYS:O	1:P:127:ALA:HB3	2.06	0.56
1:P:17:PHE:HD2	1:P:326:VAL:HG22	1.69	0.56
1:R:174:ILE:HD12	1:R:250:GLN:HG2	1.86	0.56
1:B:145:GLU:H	1:B:145:GLU:CD	2.08	0.56
1:B:36:ASN:HB3	4:B:6538:HOH:O	2.06	0.56
1:A:260:VAL:CG2	1:A:302:THR:HG21	2.36	0.56
1:A:175:LYS:CE	1:B:306:ASP:HB3	2.35	0.56
1:R:25:GLN:HE21	1:R:26:ASN:H	1.52	0.56
1:A:78:CYS:O	1:A:78:CYS:SG	2.64	0.55
1:O:324:GLN:OE1	1:O:324:GLN:HA	2.06	0.55
1:A:118:LYS:NZ	1:A:147:PHE:O	2.37	0.55
1:Q:145:GLU:CD	1:Q:145:GLU:H	2.10	0.55
1:Q:1:MET:CA	1:Q:1:MET:CE	2.85	0.55
1:R:59:ASP:H	1:R:70:ASN:HD21	1.55	0.55
1:Q:175:LYS:HD3	1:R:306:ASP:CB	2.33	0.55
1:A:138:ASN:ND2	1:A:222:VAL:HG12	2.22	0.55
1:P:143:ARG:HB2	1:P:146:ASP:OD2	2.07	0.55
1:A:1:MET:CA	1:A:1:MET:HE2	2.37	0.55
1:B:246:ASP:HA	1:B:313:ILE:HD13	1.89	0.54
1:B:144:HIS:HB2	1:B:336:LYS:O	2.07	0.54
1:O:112:ILE:HD13	1:O:148:ALA:HB1	1.89	0.54
1:Q:1:MET:CA	1:Q:1:MET:HE2	2.36	0.54
1:Q:280:ASP:HA	1:Q:299:SER:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ARG:C	1:A:336:LYS:HG2	2.28	0.54
1:A:144:HIS:HB2	1:A:336:LYS:O	2.07	0.54
1:B:182:HIS:HB3	1:B:236:ARG:HD3	1.90	0.54
1:B:87:TRP:CE3	1:B:92:ILE:HG13	2.42	0.54
1:Q:59:ASP:H	1:Q:70:ASN:HD21	1.55	0.54
1:Q:175:LYS:CE	1:Q:250:GLN:NE2	2.70	0.54
1:O:175:LYS:CE	1:O:250:GLN:NE2	2.68	0.54
1:O:209:VAL:HG22	1:O:236:ARG:HB2	1.89	0.54
1:P:87:TRP:HA	1:P:87:TRP:HE3	1.73	0.54
1:A:87:TRP:HA	1:A:87:TRP:CE3	2.43	0.54
1:A:87:TRP:HA	1:A:87:TRP:HE3	1.73	0.54
1:B:95:VAL:HG13	1:B:119:VAL:HB	1.90	0.53
1:R:175:LYS:HE3	1:R:250:GLN:NE2	2.23	0.53
1:O:106:GLU:O	1:O:109:SER:HB2	2.08	0.53
1:B:231:ASN:ND2	1:B:232:GLY:N	2.52	0.53
1:B:1:MET:CE	1:B:2:THR:H	2.22	0.53
1:Q:1:MET:C	1:Q:1:MET:CE	2.76	0.53
1:R:41:ARG:HG3	1:R:62:TYR:CZ	2.43	0.53
1:O:85:LEU:HD13	1:O:87:TRP:CZ2	2.44	0.53
1:Q:303:LEU:HD22	1:Q:304:VAL:N	2.23	0.53
1:R:85:LEU:HD13	1:R:87:TRP:CZ2	2.44	0.53
1:A:144:HIS:HD2	4:A:6343:HOH:O	1.91	0.53
1:A:298:ASP:OD1	1:B:199:ARG:NH2	2.42	0.53
1:P:87:TRP:HA	1:P:87:TRP:CE3	2.43	0.53
1:Q:175:LYS:NZ	1:R:308:ASP:OD2	2.36	0.53
1:A:142:TYR:CD2	1:A:336:LYS:HD2	2.44	0.52
1:Q:1:MET:HE3	1:Q:2:THR:N	2.24	0.52
1:P:190:ILE:CD1	1:Q:204:ALA:HB3	2.40	0.52
1:Q:134:VAL:HG23	1:Q:222:VAL:HG11	1.92	0.52
1:B:144:HIS:CD2	1:B:337:SER:HA	2.45	0.52
1:Q:89:GLU:HG2	4:Q:6781:HOH:O	2.10	0.52
1:R:152:ASN:OD1	1:R:326:VAL:HA	2.10	0.52
1:A:334:ALA:C	1:A:336:LYS:H	2.13	0.52
1:O:34:ILE:HB	1:O:76:ILE:HD13	1.91	0.52
1:Q:17:PHE:HD2	1:Q:326:VAL:HG22	1.75	0.52
1:Q:118:LYS:HE3	1:Q:147:PHE:O	2.09	0.52
1:P:82:PRO:HA	1:P:85:LEU:HD12	1.91	0.52
1:B:2:THR:HA	1:B:28:ASP:O	2.10	0.52
1:O:196:ARG:H	1:O:196:ARG:CD	2.22	0.52
1:B:25:GLN:HG2	1:B:26:ASN:N	2.21	0.52
1:R:118:LYS:HG3	1:R:148:ALA:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:17:PHE:HD2	1:R:326:VAL:HG22	1.75	0.52
1:B:193:ALA:O	1:B:201:ALA:HB1	2.10	0.51
1:B:24:ARG:HG2	1:B:24:ARG:NH2	2.25	0.51
1:O:308:ASP:OD2	1:P:175:LYS:NZ	2.43	0.51
1:O:87:TRP:CE3	1:O:92:ILE:HG13	2.46	0.51
1:R:34:ILE:HB	1:R:76:ILE:HD13	1.92	0.51
1:A:17:PHE:HD2	1:A:326:VAL:HG22	1.75	0.51
1:P:141:GLU:CG	4:P:6869:HOH:O	2.57	0.51
1:P:81:ASN:ND2	1:P:83:LEU:H	2.08	0.51
1:R:225:GLU:HG3	4:R:6773:HOH:O	2.09	0.51
1:P:323:SER:HA	1:P:326:VAL:HG13	1.92	0.51
1:P:41:ARG:HG3	1:P:62:TYR:CZ	2.45	0.51
1:A:265:GLN:O	1:A:269:GLN:HG3	2.10	0.51
1:O:146:ASP:HB3	1:O:147:PHE:CD1	2.46	0.51
1:P:25:GLN:HB2	1:P:25:GLN:NE2	2.24	0.51
1:P:213:THR:HA	2:P:4339:SO4:O2	2.11	0.51
1:A:85:LEU:HD13	1:A:87:TRP:CZ2	2.45	0.51
1:B:335:ARG:C	1:B:336:LYS:HG2	2.30	0.51
1:Q:175:LYS:HE2	1:Q:250:GLN:HE22	1.76	0.51
1:A:77:VAL:HG12	1:A:78:CYS:N	2.26	0.51
1:Q:25:GLN:HE21	1:Q:26:ASN:N	2.04	0.51
1:A:92:ILE:O	1:A:116:ALA:HA	2.11	0.50
1:A:17:PHE:CD2	1:A:326:VAL:HG22	2.46	0.50
1:Q:210:PRO:CG	1:R:315:TRP:HZ2	2.24	0.50
1:B:171:PHE:HB3	1:B:251:VAL:HG13	1.92	0.50
1:B:196:ARG:HD2	1:B:196:ARG:H	1.75	0.50
1:P:1:MET:CE	1:P:1:MET:CA	2.89	0.50
1:B:87:TRP:HA	1:B:87:TRP:CE3	2.46	0.50
1:O:204:ALA:HB3	1:R:190:ILE:HD11	1.94	0.50
1:B:87:TRP:HA	1:B:87:TRP:HE3	1.76	0.50
1:Q:199:ARG:HD2	1:Q:210:PRO:O	2.12	0.50
1:O:280:ASP:HA	1:O:299:SER:HB3	1.93	0.50
1:P:17:PHE:CD2	1:P:326:VAL:HG22	2.47	0.50
1:R:324:GLN:HA	1:R:324:GLN:OE1	2.11	0.50
1:A:134:VAL:HA	4:A:6356:HOH:O	2.11	0.50
1:P:63:ASP:OD1	1:P:64:GLU:N	2.44	0.50
1:O:247:LEU:O	1:O:311:LYS:HA	2.12	0.50
1:P:190:ILE:HG22	1:Q:186:LEU:HD23	1.93	0.49
1:O:8:ASN:OD1	1:O:35:ASN:HB3	2.11	0.49
1:B:144:HIS:HD2	4:B:6353:HOH:O	1.94	0.49
1:P:176:GLY:HA3	1:P:249:VAL:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:241:ASN:O	1:Q:242:VAL:HB	2.13	0.49
1:Q:323:SER:HA	1:Q:326:VAL:HG13	1.93	0.49
1:R:25:GLN:NE2	1:R:26:ASN:H	2.11	0.49
1:R:241:ASN:O	1:R:242:VAL:HB	2.12	0.49
1:A:241:ASN:ND2	1:A:242:VAL:H	2.10	0.49
1:Q:152:ASN:ND2	4:Q:6751:HOH:O	2.45	0.49
1:R:260:VAL:O	1:R:263:VAL:HG22	2.12	0.49
1:A:1:MET:CE	1:A:2:THR:H	2.24	0.49
1:Q:89:GLU:CD	1:Q:89:GLU:H	2.16	0.49
1:R:43:ALA:HB3	1:R:67:ILE:HD11	1.95	0.49
1:B:241:ASN:ND2	1:B:242:VAL:H	2.11	0.49
1:R:196:ARG:H	1:R:196:ARG:CD	2.24	0.49
1:B:242:VAL:CG2	1:B:285:SER:HB2	2.43	0.49
1:P:11:GLY:O	1:P:15:ARG:HG3	2.12	0.49
1:A:1:MET:CG	1:A:2:THR:H	2.23	0.49
1:B:196:ARG:N	1:B:196:ARG:NE	2.57	0.49
1:O:258:GLU:O	1:O:262:GLU:HG3	2.13	0.49
1:Q:103:VAL:HA	1:Q:121:ILE:HD13	1.95	0.49
1:R:88:LYS:N	1:R:115:GLY:HA3	2.28	0.49
1:P:25:GLN:CB	1:P:25:GLN:NE2	2.76	0.48
1:P:145:GLU:CD	1:P:145:GLU:H	2.17	0.48
1:O:175:LYS:HD3	1:P:306:ASP:HB3	1.94	0.48
1:B:126:LYS:O	1:B:127:ALA:HB3	2.14	0.48
1:B:196:ARG:HE	1:B:196:ARG:H	1.57	0.48
1:O:291:THR:HG21	1:O:296:ILE:HD11	1.95	0.48
1:A:24:ARG:NH2	1:A:328:ASP:OD1	2.46	0.48
1:P:1:MET:CE	1:P:1:MET:C	2.81	0.48
1:P:67:ILE:HD12	1:P:76:ILE:HD11	1.94	0.48
1:A:270:THR:OG1	1:A:271:THR:N	2.45	0.48
1:O:110:LYS:HG2	4:O:6701:HOH:O	2.13	0.48
1:O:255:THR:OG1	1:O:259:GLN:NE2	2.46	0.48
1:Q:161:ALA:HB3	1:Q:162:PRO:HD3	1.95	0.48
1:O:11:GLY:O	1:O:15:ARG:HG3	2.14	0.48
1:O:220:ALA:HB2	1:O:227:LYS:HA	1.96	0.48
1:P:280:ASP:HA	1:P:299:SER:HB3	1.94	0.48
1:O:144:HIS:CD2	4:O:6548:HOH:O	2.67	0.48
1:A:1:MET:HG2	1:A:2:THR:N	2.21	0.47
1:A:24:ARG:NH1	1:A:324:GLN:NE2	2.61	0.47
1:O:323:SER:HA	1:O:326:VAL:HG13	1.94	0.47
1:P:43:ALA:HB3	1:P:67:ILE:HD11	1.95	0.47
1:A:101:VAL:O	1:A:101:VAL:HG22	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:139:ASP:N	1:Q:139:ASP:OD2	2.47	0.47
1:B:95:VAL:CG1	1:B:119:VAL:HB	2.44	0.47
1:P:303:LEU:HD22	1:P:304:VAL:N	2.29	0.47
1:Q:11:GLY:HA3	3:Q:5341:NAP:O5B	2.13	0.47
1:O:152:ASN:O	1:O:153:ALA:HB3	2.14	0.47
1:O:265:GLN:O	1:O:269:GLN:HG3	2.15	0.47
1:Q:152:ASN:O	1:Q:153:ALA:HB3	2.15	0.47
1:R:167:LEU:HB3	1:R:173:ILE:HD11	1.97	0.47
1:B:196:ARG:HE	1:B:196:ARG:N	2.13	0.47
1:O:109:SER:O	1:O:113:GLN:HG3	2.15	0.47
1:P:244:VAL:HG13	1:P:244:VAL:O	2.14	0.47
1:R:265:GLN:O	1:R:269:GLN:HG3	2.14	0.47
1:A:311:LYS:NZ	4:A:6732:HOH:O	2.47	0.47
1:O:286:SER:O	1:O:289:ARG:HD3	2.15	0.47
1:O:152:ASN:OD1	1:O:326:VAL:HA	2.14	0.47
1:P:255:THR:OG1	1:P:259:GLN:NE2	2.47	0.47
1:R:255:THR:OG1	1:R:259:GLN:NE2	2.48	0.47
1:R:81:ASN:HD21	1:R:83:LEU:HD23	1.80	0.47
1:B:24:ARG:NH2	1:B:24:ARG:CG	2.75	0.47
1:B:175:LYS:NZ	1:B:250:GLN:OE1	2.48	0.47
1:B:270:THR:OG1	1:B:271:THR:N	2.46	0.47
1:O:25:GLN:NE2	1:O:26:ASN:H	2.13	0.47
1:A:95:VAL:HG13	1:A:119:VAL:HB	1.97	0.47
1:A:24:ARG:HD2	4:A:6798:HOH:O	2.15	0.47
1:A:334:ALA:O	1:A:336:LYS:N	2.46	0.47
1:A:216:ALA:HB3	1:A:231:ASN:HA	1.97	0.46
1:P:175:LYS:HE2	1:P:250:GLN:NE2	2.30	0.46
1:P:4:ARG:HD3	1:P:91:ASP:O	2.15	0.46
1:A:25:GLN:CD	1:A:25:GLN:H	2.19	0.46
1:B:191:LEU:HA	1:B:203:ALA:HB2	1.97	0.46
1:O:335:ARG:NH1	4:O:6426:HOH:O	2.48	0.46
1:P:99:THR:OG1	1:P:101:VAL:CG1	2.63	0.46
1:B:309:LEU:C	1:B:309:LEU:HD13	2.36	0.46
1:O:21:TRP:CH2	1:O:72:LYS:HE2	2.50	0.46
1:P:81:ASN:ND2	1:P:83:LEU:HB2	2.29	0.46
1:Q:176:GLY:HA3	1:Q:249:VAL:HG12	1.98	0.46
1:B:323:SER:HA	1:B:326:VAL:HG13	1.97	0.46
1:O:294:SER:HG	1:O:325:ARG:HD2	1.80	0.46
1:A:209:VAL:O	1:A:209:VAL:CG2	2.64	0.46
1:Q:220:ALA:HB2	1:Q:227:LYS:HA	1.97	0.46
1:Q:277:LYS:HD3	1:Q:296:ILE:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:87:TRP:HA	1:Q:87:TRP:HE3	1.79	0.46
1:R:19:ARG:HD3	1:R:56:PHE:CD1	2.50	0.46
1:P:112:ILE:HA	1:P:116:ALA:O	2.16	0.46
1:P:261:ASN:HA	1:P:261:ASN:HD22	1.57	0.46
1:Q:87:TRP:HA	1:Q:87:TRP:CE3	2.50	0.46
1:R:17:PHE:CD2	1:R:326:VAL:HG22	2.50	0.46
1:A:22:PHE:CZ	1:A:69:VAL:HB	2.51	0.46
1:O:101:VAL:O	1:O:101:VAL:CG2	2.63	0.46
1:R:159:CYS:HA	1:R:295:SER:HB3	1.97	0.46
1:A:25:GLN:NE2	1:A:25:GLN:H	2.13	0.46
1:B:106:GLU:HG3	4:B:6605:HOH:O	2.15	0.46
1:P:294:SER:OG	1:P:325:ARG:HD2	2.16	0.46
1:P:45:HIS:CD2	1:Q:198:LEU:HG	2.50	0.46
1:Q:209:VAL:HA	1:Q:210:PRO:HD3	1.77	0.46
1:R:3:ILE:CD1	1:R:334:ALA:HB2	2.46	0.46
1:A:241:ASN:O	1:A:242:VAL:HG13	2.15	0.46
1:B:11:GLY:O	1:B:15:ARG:HG3	2.16	0.46
1:O:303:LEU:CD1	1:O:305:MET:HG2	2.46	0.46
1:P:18:LEU:HD22	1:P:22:PHE:CD1	2.51	0.46
1:Q:247:LEU:O	1:Q:311:LYS:HA	2.15	0.46
1:O:327:VAL:O	1:O:331:GLU:HG2	2.16	0.45
1:Q:165:LYS:HB2	1:Q:223:ILE:HD11	1.98	0.45
1:R:118:LYS:NZ	1:R:144:HIS:O	2.49	0.45
1:B:34:ILE:HB	1:B:76:ILE:HD13	1.97	0.45
1:B:77:VAL:HG12	1:B:78:CYS:N	2.32	0.45
1:O:139:ASP:N	1:O:139:ASP:OD2	2.49	0.45
1:R:18:LEU:HD22	1:R:22:PHE:CE1	2.51	0.45
1:O:294:SER:OG	1:O:325:ARG:HD2	2.15	0.45
1:O:25:GLN:HE21	1:O:26:ASN:H	1.64	0.45
1:P:35:ASN:ND2	3:P:4341:NAP:H2A	2.32	0.45
1:R:139:ASP:N	1:R:139:ASP:OD2	2.50	0.45
1:R:280:ASP:HA	1:R:299:SER:HB3	1.98	0.45
1:B:107:GLY:O	1:B:110:LYS:HG3	2.16	0.45
1:O:231:ASN:HB2	1:P:305:MET:SD	2.56	0.45
1:A:24:ARG:NH1	1:A:324:GLN:HE22	2.15	0.45
1:B:1:MET:HB3	1:B:2:THR:H	1.44	0.45
1:P:19:ARG:CZ	1:P:56:PHE:HB2	2.46	0.45
1:P:184:TYR:CE1	1:Q:191:LEU:HD21	2.52	0.45
1:P:184:TYR:HE1	1:Q:191:LEU:HD21	1.80	0.45
1:O:261:ASN:HA	1:O:261:ASN:HD22	1.59	0.45
1:P:209:VAL:HA	1:P:210:PRO:HD3	1.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:87:TRP:HE3	1:R:87:TRP:HA	1.82	0.45
1:A:123:ALA:HB2	3:A:1341:NAP:H1D	1.98	0.45
1:A:34:ILE:HB	1:A:76:ILE:HD13	1.99	0.45
1:B:127:ALA:HB3	4:B:6696:HOH:O	2.17	0.45
1:P:303:LEU:HD11	1:P:305:MET:HG2	1.99	0.45
1:P:81:ASN:HD22	1:P:81:ASN:C	2.20	0.45
1:P:94:LEU:HA	1:P:118:LYS:O	2.17	0.45
1:A:94:LEU:HD12	1:A:118:LYS:O	2.17	0.45
1:A:199:ARG:HH22	1:B:298:ASP:CG	2.21	0.45
1:O:103:VAL:HA	1:O:121:ILE:HD13	1.99	0.45
1:O:134:VAL:HG23	1:O:222:VAL:HG11	1.99	0.45
1:P:249:VAL:HG23	1:P:310:VAL:HG22	1.99	0.45
1:R:81:ASN:HD21	1:R:83:LEU:HD22	1.82	0.45
1:A:144:HIS:CD2	4:A:6343:HOH:O	2.68	0.44
1:B:89:GLU:OE1	1:B:89:GLU:N	2.43	0.44
1:R:161:ALA:HB3	1:R:162:PRO:HD3	1.99	0.44
1:P:220:ALA:HB2	1:P:227:LYS:HA	1.99	0.44
1:B:56:PHE:CD2	1:B:60:ILE:HD11	2.53	0.44
1:B:78:CYS:O	1:B:78:CYS:SG	2.76	0.44
1:Q:17:PHE:CD2	1:Q:326:VAL:HG22	2.51	0.44
1:A:184:TYR:HA	1:A:188:GLN:OE1	2.18	0.44
1:Q:112:ILE:CD1	1:Q:148:ALA:HB1	2.48	0.44
1:A:101:VAL:O	1:A:101:VAL:CG2	2.65	0.44
1:O:81:ASN:C	1:O:81:ASN:HD22	2.21	0.44
1:P:191:LEU:HD21	1:Q:184:TYR:CE1	2.53	0.44
1:B:17:PHE:HD2	1:B:326:VAL:HG22	1.83	0.44
1:O:103:VAL:HG23	1:O:126:LYS:HB2	1.98	0.44
1:P:168:HIS:HB2	1:P:173:ILE:HG12	2.00	0.44
1:Q:261:ASN:HD22	1:Q:261:ASN:HA	1.60	0.44
1:R:95:VAL:HG13	1:R:119:VAL:HB	1.99	0.44
1:B:25:GLN:NE2	1:B:25:GLN:H	2.16	0.44
1:Q:255:THR:OG1	1:Q:256:ILE:N	2.50	0.44
1:R:332:LEU:CD2	1:R:336:LYS:HD3	2.48	0.44
1:R:99:THR:OG1	1:R:101:VAL:CG1	2.66	0.44
1:O:231:ASN:HA	1:O:231:ASN:HD22	1.47	0.44
1:P:88:LYS:N	1:P:115:GLY:HA3	2.33	0.44
1:A:106:GLU:HG3	4:A:6718:HOH:O	2.16	0.43
1:B:332:LEU:HD22	1:B:336:LYS:HD2	1.99	0.43
1:B:36:ASN:CB	4:B:6538:HOH:O	2.65	0.43
1:O:303:LEU:HD11	1:O:305:MET:HG2	2.00	0.43
1:P:1:MET:CE	1:P:1:MET:H3	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:11:GLY:HA3	3:P:4341:NAP:O5B	2.18	0.43
1:R:87:TRP:CE3	1:R:87:TRP:HA	2.53	0.43
1:P:10:PHE:CZ	1:P:18:LEU:HD12	2.53	0.43
1:R:159:CYS:O	1:R:162:PRO:HD2	2.18	0.43
1:R:294:SER:OG	1:R:325:ARG:HD2	2.18	0.43
1:A:260:VAL:HG22	1:A:302:THR:HG21	1.99	0.43
1:B:209:VAL:O	1:B:209:VAL:CG2	2.67	0.43
1:O:126:LYS:O	1:O:127:ALA:CB	2.66	0.43
1:P:265:GLN:O	1:P:269:GLN:HG3	2.18	0.43
1:B:24:ARG:HE	1:B:324:GLN:HE22	1.67	0.43
1:P:103:VAL:HA	1:P:121:ILE:HD13	2.00	0.43
1:P:255:THR:OG1	1:P:256:ILE:N	2.51	0.43
1:R:64:GLU:HB2	4:R:6713:HOH:O	2.18	0.43
1:A:168:HIS:HA	1:A:173:ILE:HG13	1.98	0.43
1:A:196:ARG:CD	4:A:6769:HOH:O	2.60	0.43
1:B:94:LEU:HD12	1:B:118:LYS:O	2.19	0.43
1:P:270:THR:OG1	1:P:271:THR:N	2.51	0.43
1:A:99:THR:OG1	1:A:101:VAL:HG12	2.18	0.43
1:P:225:GLU:HG3	4:P:6458:HOH:O	2.18	0.43
1:A:261:ASN:HA	1:A:261:ASN:HD22	1.63	0.43
1:Q:34:ILE:HB	1:Q:76:ILE:HD13	2.00	0.43
1:P:231:ASN:HA	1:P:231:ASN:HD22	1.54	0.43
1:R:209:VAL:HG22	1:R:236:ARG:HB2	2.00	0.43
1:B:139:ASP:OD2	1:B:139:ASP:N	2.47	0.43
1:B:41:ARG:HG3	1:B:62:TYR:CZ	2.54	0.43
1:Q:99:THR:OG1	1:Q:101:VAL:CG1	2.65	0.43
1:B:22:PHE:CZ	1:B:69:VAL:HB	2.54	0.43
1:P:190:ILE:O	1:P:191:LEU:HD23	2.19	0.43
1:A:190:ILE:H	1:A:190:ILE:HG13	1.55	0.42
1:O:99:THR:OG1	1:O:101:VAL:HG12	2.19	0.42
1:O:17:PHE:HD2	1:O:326:VAL:HG22	1.84	0.42
1:P:94:LEU:HD12	1:P:118:LYS:O	2.18	0.42
1:P:100:GLY:HA2	3:P:4341:NAP:O3D	2.19	0.42
1:P:82:PRO:HA	1:P:85:LEU:CD1	2.49	0.42
1:A:174:ILE:HD12	1:A:250:GLN:HG2	2.00	0.42
1:Q:5:VAL:CG1	1:Q:96:ILE:HD13	2.49	0.42
1:R:134:VAL:HG23	1:R:222:VAL:HG11	2.01	0.42
1:R:241:ASN:O	1:R:242:VAL:CB	2.67	0.42
1:R:176:GLY:HA3	1:R:249:VAL:HG12	2.00	0.42
1:R:19:ARG:CZ	1:R:56:PHE:HB2	2.50	0.42
1:A:100:GLY:HA2	3:A:1341:NAP:O3D	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:174:ILE:HD12	1:O:250:GLN:HG2	2.00	0.42
1:P:18:LEU:HD22	1:P:22:PHE:CE1	2.54	0.42
1:P:303:LEU:CD1	1:P:305:MET:HG2	2.48	0.42
1:Q:210:PRO:CG	1:R:315:TRP:CZ2	3.02	0.42
1:Q:87:TRP:CE3	1:Q:92:ILE:HG13	2.55	0.42
1:R:81:ASN:C	1:R:81:ASN:HD22	2.22	0.42
1:A:63:ASP:OD2	1:A:63:ASP:C	2.57	0.42
1:P:191:LEU:HD21	1:Q:184:TYR:HE1	1.83	0.42
1:Q:243:SER:HB2	1:Q:316:TYR:CZ	2.54	0.42
1:A:171:PHE:HB3	1:A:251:VAL:HG13	1.98	0.42
1:B:334:ALA:C	1:B:336:LYS:H	2.23	0.42
1:P:139:ASP:N	1:P:139:ASP:OD2	2.53	0.42
1:A:242:VAL:HG21	1:A:285:SER:O	2.20	0.42
1:A:24:ARG:CD	4:A:6798:HOH:O	2.68	0.42
1:P:247:LEU:O	1:P:311:LYS:HA	2.20	0.42
1:Q:78:CYS:O	1:Q:78:CYS:SG	2.78	0.42
1:B:209:VAL:HA	1:B:210:PRO:HD3	1.77	0.42
1:P:152:ASN:OD1	1:P:326:VAL:HA	2.20	0.42
1:A:158:ASN:ND2	4:A:6507:HOH:O	2.53	0.42
1:O:10:PHE:CZ	1:O:18:LEU:HD12	2.55	0.42
1:O:81:ASN:ND2	1:O:83:LEU:H	2.18	0.42
1:P:291:THR:HG21	1:P:296:ILE:HD11	2.02	0.42
1:Q:112:ILE:HD13	1:Q:148:ALA:HB1	2.01	0.42
1:Q:209:VAL:HB	1:R:284:VAL:HG12	2.02	0.42
1:A:251:VAL:CG1	1:A:252:GLU:N	2.82	0.42
1:Q:88:LYS:HE2	1:Q:115:GLY:HA2	2.02	0.42
1:Q:89:GLU:N	1:Q:89:GLU:CD	2.74	0.42
1:R:175:LYS:CE	1:R:250:GLN:NE2	2.83	0.42
1:R:296:ILE:O	1:R:314:ALA:HA	2.20	0.42
1:R:325:ARG:NE	1:R:325:ARG:HA	2.35	0.42
1:A:242:VAL:CG2	1:A:285:SER:HB2	2.50	0.41
1:A:48:GLU:O	1:A:55:ARG:HA	2.20	0.41
1:B:135:ILE:HG12	4:B:6368:HOH:O	2.20	0.41
1:B:199:ARG:HH21	1:B:210:PRO:HG2	1.85	0.41
1:R:103:VAL:HA	1:R:121:ILE:HD13	2.02	0.41
1:R:258:GLU:O	1:R:262:GLU:HG3	2.20	0.41
1:R:327:VAL:O	1:R:331:GLU:HG2	2.20	0.41
1:B:63:ASP:OD2	1:B:63:ASP:C	2.58	0.41
1:Q:260:VAL:HG22	1:Q:302:THR:HG21	2.01	0.41
1:A:303:LEU:HD23	1:A:304:VAL:N	2.34	0.41
1:O:118:LYS:NZ	1:O:144:HIS:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:277:LYS:HD3	1:P:296:ILE:HG23	2.03	0.41
1:B:158:ASN:ND2	4:B:6431:HOH:O	2.53	0.41
1:B:260:VAL:HG21	1:B:302:THR:HG21	1.98	0.41
1:Q:97:GLU:OE2	1:Q:99:THR:HG23	2.20	0.41
1:R:220:ALA:HB2	1:R:227:LYS:HA	2.03	0.41
1:O:39:ASP:OD1	1:O:41:ARG:HB3	2.20	0.41
1:O:95:VAL:HG13	1:O:119:VAL:HB	2.03	0.41
1:P:190:ILE:HD11	1:Q:204:ALA:CB	2.49	0.41
1:Q:18:LEU:HD22	1:Q:22:PHE:CE1	2.55	0.41
1:R:277:LYS:HD3	1:R:296:ILE:HG23	2.01	0.41
1:P:85:LEU:HD13	1:P:87:TRP:CZ2	2.56	0.41
1:Q:178:MET:HE3	1:Q:178:MET:O	2.21	0.41
1:A:119:VAL:HG13	1:A:149:VAL:HG22	2.01	0.41
1:A:335:ARG:O	1:A:336:LYS:CB	2.68	0.41
1:B:41:ARG:HG3	1:B:62:TYR:OH	2.20	0.41
1:P:175:LYS:CE	1:P:250:GLN:HE22	2.33	0.41
1:P:81:ASN:HD22	1:P:83:LEU:H	1.67	0.41
1:A:323:SER:HA	1:A:326:VAL:CG1	2.46	0.41
1:A:209:VAL:HA	1:A:210:PRO:HD3	1.79	0.41
1:O:205:ALA:HB3	4:O:6640:HOH:O	2.19	0.41
1:P:1:MET:HE2	1:P:1:MET:CA	2.51	0.41
1:P:209:VAL:CG2	1:P:209:VAL:O	2.69	0.41
1:P:159:CYS:SG	1:P:295:SER:HB3	2.61	0.41
1:Q:11:GLY:O	1:Q:15:ARG:HG3	2.19	0.41
1:Q:19:ARG:HD3	1:Q:56:PHE:CD1	2.55	0.41
1:A:20:CYS:HB3	1:A:324:GLN:NE2	2.36	0.41
1:O:209:VAL:HA	1:O:210:PRO:HD3	1.81	0.41
1:O:241:ASN:O	1:O:242:VAL:HB	2.21	0.41
1:P:161:ALA:HB3	1:P:162:PRO:HD3	2.02	0.41
1:R:231:ASN:HA	1:R:231:ASN:HD22	1.53	0.41
4:A:6732:HOH:O	1:B:177:THR:HG23	2.19	0.40
1:Q:305:MET:HB2	1:Q:309:LEU:HB3	2.03	0.40
1:A:315:TRP:HZ2	1:B:210:PRO:CG	2.35	0.40
1:A:59:ASP:O	1:A:69:VAL:HA	2.20	0.40
1:B:260:VAL:HG22	1:B:302:THR:HG21	2.03	0.40
1:P:184:TYR:HA	1:P:188:GLN:OE1	2.21	0.40
1:P:291:THR:HG21	1:P:296:ILE:CD1	2.52	0.40
1:P:260:VAL:HG22	1:P:302:THR:HG21	2.01	0.40
1:P:34:ILE:HB	1:P:76:ILE:HD13	2.03	0.40
1:Q:124:PRO:HG3	1:Q:154:SER:HB3	2.02	0.40
1:A:309:LEU:C	1:A:309:LEU:CD1	2.89	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:VAL:HG21	1:B:285:SER:HB2	2.04	0.40
1:P:112:ILE:HG23	1:P:116:ALA:O	2.21	0.40
1:Q:35:ASN:HA	1:Q:77:VAL:O	2.22	0.40
1:R:146:ASP:HB3	1:R:147:PHE:CD1	2.57	0.40
1:Q:167:LEU:HB3	1:Q:173:ILE:HD11	2.03	0.40
1:R:35:ASN:HA	1:R:77:VAL:O	2.22	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	336/380 (88%)	308 (92%)	22 (6%)	6 (2%)	10	17
1	B	336/380 (88%)	308 (92%)	22 (6%)	6 (2%)	10	17
1	O	336/380 (88%)	313 (93%)	20 (6%)	3 (1%)	20	36
1	P	336/380 (88%)	318 (95%)	16 (5%)	2 (1%)	28	48
1	Q	336/380 (88%)	314 (94%)	18 (5%)	4 (1%)	15	27
1	R	336/380 (88%)	313 (93%)	21 (6%)	2 (1%)	28	48
All	All	2016/2280 (88%)	1874 (93%)	119 (6%)	23 (1%)	17	29

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	336	LYS
1	A	242	VAL
1	B	242	VAL
1	B	336	LYS
1	O	242	VAL
1	P	242	VAL

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Mol	Chain	Res	Type
1	Q	242	VAL
1	R	242	VAL
1	A	203	ALA
1	B	127	ALA
1	O	172	GLY
1	Q	172	GLY
1	A	127	ALA
1	A	335	ARG
1	O	127	ALA
1	R	172	GLY
1	B	335	ARG
1	Q	127	ALA
1	P	172	GLY
1	Q	186	LEU
1	B	238	PRO
1	B	172	GLY
1	A	172	GLY

### 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	284/321 (88%)	254 (89%)	30 (11%)	8	15
1	B	284/321 (88%)	256 (90%)	28 (10%)	9	17
1	O	284/321 (88%)	262 (92%)	22 (8%)	15	28
1	P	284/321 (88%)	260 (92%)	24 (8%)	12	23
1	Q	284/321 (88%)	264 (93%)	20 (7%)	18	33
1	R	284/321 (88%)	262 (92%)	22 (8%)	15	28
All	All	1704/1926 (88%)	1558 (91%)	146 (9%)	12	23

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET

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Mol	Chain	Res	Type
1	A	18	LEU
1	A	25	GLN
1	A	36	ASN
1	A	37	THR
1	A	39	ASP
1	A	57	ASN
1	A	80	ARG
1	A	87	TRP
1	A	89	GLU
1	A	97	GLU
1	A	119	VAL
1	A	130	VAL
1	A	145	GLU
1	A	167	LEU
1	A	190	ILE
1	A	196	ARG
1	A	198	LEU
1	A	209	VAL
1	A	219	VAL
1	A	231	ASN
1	A	242	VAL
1	A	260	VAL
1	A	305	MET
1	A	310	VAL
1	A	312	VAL
1	A	324	GLN
1	A	326	VAL
1	A	332	LEU
1	A	336	LYS
1	B	18	LEU
1	B	24	ARG
1	B	25	GLN
1	B	36	ASN
1	B	87	TRP
1	B	89	GLU
1	B	119	VAL
1	B	120	LEU
1	B	130	VAL
1	B	143	ARG
1	B	145	GLU
1	B	155	CYS
1	B	167	LEU

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Mol	Chain	Res	Type
1	B	178	MET
1	B	189	ARG
1	B	190	ILE
1	B	196	ARG
1	B	198	LEU
1	B	209	VAL
1	B	219	VAL
1	B	231	ASN
1	B	242	VAL
1	B	300	SER
1	B	305	MET
1	B	312	VAL
1	B	324	GLN
1	B	332	LEU
1	B	336	LYS
1	O	1	MET
1	O	18	LEU
1	O	25	GLN
1	O	63	ASP
1	O	72	LYS
1	O	79	ASP
1	O	81	ASN
1	O	83	LEU
1	O	87	TRP
1	O	95	VAL
1	O	117	LYS
1	O	119	VAL
1	O	126	LYS
1	O	145	GLU
1	O	152	ASN
1	O	178	MET
1	O	196	ARG
1	O	231	ASN
1	O	240	PRO
1	O	260	VAL
1	O	324	GLN
1	O	332	LEU
1	P	1	MET
1	P	2	THR
1	P	18	LEU
1	P	25	GLN
1	P	39	ASP

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Mol	Chain	Res	Type
1	P	63	ASP
1	P	79	ASP
1	P	81	ASN
1	P	83	LEU
1	P	87	TRP
1	P	95	VAL
1	P	96	ILE
1	P	119	VAL
1	P	145	GLU
1	P	152	ASN
1	P	178	MET
1	P	196	ARG
1	P	198	LEU
1	P	209	VAL
1	P	231	ASN
1	P	252	GLU
1	P	261	ASN
1	P	332	LEU
1	P	336	LYS
1	Q	1	MET
1	Q	18	LEU
1	Q	25	GLN
1	Q	63	ASP
1	Q	79	ASP
1	Q	81	ASN
1	Q	83	LEU
1	Q	87	TRP
1	Q	95	VAL
1	Q	119	VAL
1	Q	145	GLU
1	Q	152	ASN
1	Q	178	MET
1	Q	196	ARG
1	Q	198	LEU
1	Q	209	VAL
1	Q	231	ASN
1	Q	240	PRO
1	Q	260	VAL
1	Q	332	LEU
1	R	1	MET
1	R	18	LEU
1	R	25	GLN

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Mol	Chain	Res	Type
1	R	63	ASP
1	R	79	ASP
1	R	81	ASN
1	R	83	LEU
1	R	87	TRP
1	R	95	VAL
1	R	96	ILE
1	R	119	VAL
1	R	145	GLU
1	R	152	ASN
1	R	155	CYS
1	R	178	MET
1	R	196	ARG
1	R	231	ASN
1	R	260	VAL
1	R	300	SER
1	R	316	TYR
1	R	332	LEU
1	R	336	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (72) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	26	ASN
1	A	36	ASN
1	A	57	ASN
1	A	70	ASN
1	A	144	HIS
1	A	158	ASN
1	A	231	ASN
1	A	241	ASN
1	A	261	ASN
1	A	324	GLN
1	B	25	GLN
1	B	36	ASN
1	B	57	ASN
1	B	70	ASN
1	B	84	ASN
1	B	144	HIS
1	B	158	ASN
1	B	231	ASN

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Mol	Chain	Res	Type
1	B	241	ASN
1	B	261	ASN
1	B	324	GLN
1	O	25	GLN
1	O	57	ASN
1	O	70	ASN
1	O	81	ASN
1	O	84	ASN
1	O	144	HIS
1	O	158	ASN
1	O	231	ASN
1	O	259	GLN
1	O	261	ASN
1	O	265	GLN
1	P	25	GLN
1	P	26	ASN
1	P	45	HIS
1	P	57	ASN
1	P	70	ASN
1	P	81	ASN
1	P	84	ASN
1	P	113	GLN
1	P	144	HIS
1	P	158	ASN
1	P	231	ASN
1	P	250	GLN
1	P	259	GLN
1	P	261	ASN
1	P	265	GLN
1	Q	25	GLN
1	Q	57	ASN
1	Q	70	ASN
1	Q	81	ASN
1	Q	113	GLN
1	Q	144	HIS
1	Q	152	ASN
1	Q	158	ASN
1	Q	250	GLN
1	Q	259	GLN
1	Q	261	ASN
1	Q	265	GLN
1	R	25	GLN

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Mol	Chain	Res	Type
1	R	57	ASN
1	R	70	ASN
1	R	81	ASN
1	R	84	ASN
1	R	113	GLN
1	R	144	HIS
1	R	158	ASN
1	R	231	ASN
1	R	259	GLN
1	R	261	ASN
1	R	265	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

18 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	$\# Z  > 2$
2	SO4	A	1339	-	4,4,4	0.38	0	6,6,6	0.36	0
2	SO4	A	1340	-	4,4,4	0.16	0	6,6,6	0.15	0
3	NAP	A	1341	-	44,52,52	1.97	12 (27%)	51,80,80	1.86	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	B	2339	-	4,4,4	0.26	0	6,6,6	0.26	0
2	SO4	B	2340	-	4,4,4	0.15	0	6,6,6	0.33	0
3	NAP	B	2341	-	44,52,52	1.83	9 (20%)	51,80,80	1.81	10 (19%)
2	SO4	O	3339	-	4,4,4	0.36	0	6,6,6	0.25	0
2	SO4	O	3340	-	4,4,4	0.34	0	6,6,6	0.26	0
3	NAP	O	3341	-	44,52,52	1.99	11 (25%)	51,80,80	1.78	12 (23%)
2	SO4	P	4339	-	4,4,4	0.23	0	6,6,6	0.38	0
2	SO4	P	4340	-	4,4,4	0.25	0	6,6,6	0.23	0
3	NAP	P	4341	-	44,52,52	1.93	12 (27%)	51,80,80	1.63	11 (21%)
2	SO4	Q	5339	-	4,4,4	0.29	0	6,6,6	0.18	0
2	SO4	Q	5340	-	4,4,4	0.22	0	6,6,6	0.26	0
3	NAP	Q	5341	-	44,52,52	1.94	11 (25%)	51,80,80	1.75	12 (23%)
2	SO4	R	6339	-	4,4,4	0.36	0	6,6,6	0.16	0
2	SO4	R	6340	-	4,4,4	0.23	0	6,6,6	0.26	0
3	NAP	R	6341	-	44,52,52	1.85	11 (25%)	51,80,80	1.74	12 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1339	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1340	-	-	0/0/0/0	0/0/0/0
3	NAP	A	1341	-	-	0/27/67/67	0/5/5/5
2	SO4	B	2339	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2340	-	-	0/0/0/0	0/0/0/0
3	NAP	B	2341	-	-	0/27/67/67	0/5/5/5
2	SO4	O	3339	-	-	0/0/0/0	0/0/0/0
2	SO4	O	3340	-	-	0/0/0/0	0/0/0/0
3	NAP	O	3341	-	-	0/27/67/67	0/5/5/5
2	SO4	P	4339	-	-	0/0/0/0	0/0/0/0
2	SO4	P	4340	-	-	0/0/0/0	0/0/0/0
3	NAP	P	4341	-	-	0/27/67/67	0/5/5/5
2	SO4	Q	5339	-	-	0/0/0/0	0/0/0/0
2	SO4	Q	5340	-	-	0/0/0/0	0/0/0/0
3	NAP	Q	5341	-	-	0/27/67/67	0/5/5/5
2	SO4	R	6339	-	-	0/0/0/0	0/0/0/0
2	SO4	R	6340	-	-	0/0/0/0	0/0/0/0
3	NAP	R	6341	-	-	0/27/67/67	0/5/5/5

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	3341	NAP	C2D-C1D	-4.61	1.46	1.53
3	B	2341	NAP	C2D-C1D	-4.51	1.46	1.53
3	Q	5341	NAP	C2D-C1D	-3.88	1.47	1.53
3	R	6341	NAP	C2D-C1D	-3.60	1.47	1.53
3	A	1341	NAP	PA-O1A	-3.30	1.38	1.50
3	A	1341	NAP	C2D-C1D	-3.07	1.48	1.53
3	P	4341	NAP	PA-O1A	-2.78	1.40	1.50
3	Q	5341	NAP	PA-O1A	-2.74	1.40	1.50
3	R	6341	NAP	PA-O1A	-2.41	1.41	1.50
3	P	4341	NAP	C2D-C1D	-2.35	1.49	1.53
3	O	3341	NAP	PA-O1A	-2.26	1.42	1.50
3	B	2341	NAP	PA-O1A	-2.09	1.43	1.50
3	R	6341	NAP	C5B-C4B	2.02	1.58	1.51
3	R	6341	NAP	C3N-C7N	2.04	1.53	1.50
3	B	2341	NAP	P2B-O2B	2.14	1.63	1.59
3	O	3341	NAP	C6N-C5N	2.16	1.43	1.38
3	P	4341	NAP	P2B-O2B	2.21	1.63	1.59
3	O	3341	NAP	O4B-C4B	2.28	1.50	1.45
3	A	1341	NAP	C3B-C4B	2.29	1.59	1.53
3	A	1341	NAP	C3D-C4D	2.30	1.59	1.53
3	P	4341	NAP	O4B-C4B	2.34	1.50	1.45
3	P	4341	NAP	C5N-C4N	2.38	1.43	1.38
3	Q	5341	NAP	C5N-C4N	2.39	1.43	1.38
3	A	1341	NAP	P2B-O2B	2.40	1.63	1.59
3	R	6341	NAP	C4A-N3A	2.41	1.39	1.35
3	R	6341	NAP	O4B-C4B	2.43	1.50	1.45
3	A	1341	NAP	C4A-N3A	2.49	1.39	1.35
3	B	2341	NAP	C6N-N1N	2.67	1.42	1.35
3	A	1341	NAP	C5N-C4N	2.67	1.44	1.38
3	P	4341	NAP	C3N-C7N	2.72	1.54	1.50
3	P	4341	NAP	C4A-N3A	2.91	1.39	1.35
3	Q	5341	NAP	C4A-N3A	2.93	1.39	1.35
3	O	3341	NAP	C4A-N3A	3.02	1.40	1.35
3	Q	5341	NAP	C3N-C7N	3.05	1.55	1.50
3	Q	5341	NAP	C6N-N1N	3.07	1.43	1.35
3	R	6341	NAP	C6N-N1N	3.10	1.43	1.35
3	B	2341	NAP	O4D-C1D	3.14	1.45	1.41
3	A	1341	NAP	C6N-N1N	3.21	1.43	1.35
3	Q	5341	NAP	P2B-O2B	3.24	1.65	1.59
3	A	1341	NAP	C2A-N1A	3.29	1.40	1.33
3	O	3341	NAP	P2B-O2B	3.31	1.65	1.59
3	B	2341	NAP	C2A-N1A	3.33	1.40	1.33
3	P	4341	NAP	C6N-N1N	3.44	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	3341	NAP	C6N-N1N	3.48	1.44	1.35
3	O	3341	NAP	O4D-C1D	3.53	1.46	1.41
3	Q	5341	NAP	C2A-N3A	3.62	1.38	1.32
3	Q	5341	NAP	C2A-N1A	3.80	1.41	1.33
3	B	2341	NAP	C4A-N3A	3.85	1.41	1.35
3	P	4341	NAP	C2A-N1A	3.87	1.41	1.33
3	O	3341	NAP	C2A-N1A	4.07	1.41	1.33
3	R	6341	NAP	C2A-N1A	4.11	1.41	1.33
3	R	6341	NAP	C2A-N3A	4.14	1.39	1.32
3	P	4341	NAP	O4D-C1D	4.24	1.47	1.41
3	R	6341	NAP	O4D-C1D	4.35	1.47	1.41
3	B	2341	NAP	C4N-C3N	4.37	1.46	1.39
3	A	1341	NAP	C2A-N3A	4.46	1.39	1.32
3	O	3341	NAP	C2A-N3A	4.50	1.39	1.32
3	Q	5341	NAP	C4N-C3N	4.61	1.46	1.39
3	Q	5341	NAP	O4D-C1D	4.64	1.47	1.41
3	P	4341	NAP	C2A-N3A	4.66	1.39	1.32
3	B	2341	NAP	C2A-N3A	4.66	1.39	1.32
3	R	6341	NAP	C4N-C3N	4.80	1.47	1.39
3	A	1341	NAP	O4D-C1D	4.99	1.48	1.41
3	A	1341	NAP	C4N-C3N	5.02	1.47	1.39
3	P	4341	NAP	C4N-C3N	5.09	1.47	1.39
3	O	3341	NAP	C4N-C3N	5.52	1.48	1.39

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1341	NAP	N3A-C2A-N1A	-7.06	122.71	128.86
3	B	2341	NAP	N3A-C2A-N1A	-6.82	122.91	128.86
3	P	4341	NAP	N3A-C2A-N1A	-6.80	122.93	128.86
3	Q	5341	NAP	N3A-C2A-N1A	-6.76	122.97	128.86
3	O	3341	NAP	N3A-C2A-N1A	-6.62	123.09	128.86
3	R	6341	NAP	N3A-C2A-N1A	-6.55	123.15	128.86
3	B	2341	NAP	C1B-N9A-C4A	-3.59	120.43	126.64
3	A	1341	NAP	C1B-N9A-C4A	-3.39	120.77	126.64
3	O	3341	NAP	O7N-C7N-C3N	-3.37	115.68	119.62
3	B	2341	NAP	O7N-C7N-C3N	-3.32	115.74	119.62
3	A	1341	NAP	O7N-C7N-C3N	-3.28	115.79	119.62
3	B	2341	NAP	C3N-C2N-N1N	-3.23	117.17	120.43
3	O	3341	NAP	C3N-C2N-N1N	-3.12	117.29	120.43
3	R	6341	NAP	C1B-N9A-C4A	-2.92	121.59	126.64
3	Q	5341	NAP	C1B-N9A-C4A	-2.91	121.61	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	5341	NAP	O5B-C5B-C4B	-2.71	99.41	109.00
3	R	6341	NAP	O7N-C7N-C3N	-2.69	116.47	119.62
3	P	4341	NAP	C1B-N9A-C4A	-2.61	122.13	126.64
3	O	3341	NAP	O5B-C5B-C4B	-2.58	99.86	109.00
3	A	1341	NAP	C3N-C2N-N1N	-2.57	117.84	120.43
3	Q	5341	NAP	O7N-C7N-C3N	-2.48	116.72	119.62
3	O	3341	NAP	C1B-N9A-C4A	-2.45	122.40	126.64
3	P	4341	NAP	O5B-C5B-C4B	-2.45	100.32	109.00
3	A	1341	NAP	O5B-C5B-C4B	-2.42	100.41	109.00
3	B	2341	NAP	O5B-C5B-C4B	-2.42	100.43	109.00
3	P	4341	NAP	O4B-C1B-C2B	-2.31	102.56	106.59
3	R	6341	NAP	C3N-C2N-N1N	-2.27	118.14	120.43
3	Q	5341	NAP	C5N-C6N-N1N	-2.20	117.03	120.40
3	O	3341	NAP	O4B-C1B-C2B	-2.17	102.80	106.59
3	Q	5341	NAP	O4B-C1B-C2B	-2.14	102.84	106.59
3	P	4341	NAP	O3B-C3B-C4B	-2.14	104.84	111.09
3	R	6341	NAP	O5B-C5B-C4B	-2.12	101.50	109.00
3	A	1341	NAP	O4B-C4B-C3B	-2.09	101.01	105.17
3	R	6341	NAP	O4B-C1B-C2B	-2.02	103.05	106.59
3	Q	5341	NAP	O3X-P2B-O2X	2.04	115.83	107.61
3	A	1341	NAP	O3X-P2B-O2X	2.05	115.88	107.61
3	P	4341	NAP	C4B-O4B-C1B	2.10	112.00	109.77
3	P	4341	NAP	C3N-C7N-N7N	2.19	120.28	117.77
3	O	3341	NAP	O3X-P2B-O2X	2.20	116.48	107.61
3	R	6341	NAP	O3X-P2B-O2X	2.28	116.80	107.61
3	P	4341	NAP	O3X-P2B-O2X	2.31	116.94	107.61
3	Q	5341	NAP	C4B-O4B-C1B	2.38	112.31	109.77
3	P	4341	NAP	C2N-C3N-C4N	2.45	121.05	118.26
3	O	3341	NAP	C4B-O4B-C1B	2.46	112.38	109.77
3	Q	5341	NAP	C2N-C3N-C4N	2.50	121.11	118.26
3	R	6341	NAP	O2A-PA-O1A	2.59	125.70	112.28
3	B	2341	NAP	O2A-PA-O1A	2.63	125.89	112.28
3	O	3341	NAP	O2A-PA-O1A	2.66	126.07	112.28
3	P	4341	NAP	O2A-PA-O1A	2.74	126.44	112.28
3	R	6341	NAP	C4B-O4B-C1B	2.75	112.69	109.77
3	Q	5341	NAP	O2A-PA-O1A	2.80	126.80	112.28
3	A	1341	NAP	C5A-C6A-N6A	2.83	126.23	120.47
3	P	4341	NAP	C5A-C6A-N6A	2.86	126.30	120.47
3	A	1341	NAP	C4B-O4B-C1B	2.90	112.85	109.77
3	B	2341	NAP	C4B-O4B-C1B	2.91	112.86	109.77
3	R	6341	NAP	C2N-C3N-C4N	2.91	121.58	118.26
3	A	1341	NAP	C2N-C3N-C4N	3.00	121.68	118.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2341	NAP	C5A-C6A-N6A	3.01	126.60	120.47
3	B	2341	NAP	C2N-C3N-C4N	3.04	121.73	118.26
3	R	6341	NAP	C3N-C7N-N7N	3.07	121.28	117.77
3	A	1341	NAP	O2A-PA-O1A	3.07	128.17	112.28
3	Q	5341	NAP	C3N-C7N-N7N	3.09	121.30	117.77
3	O	3341	NAP	C5A-C6A-N6A	3.13	126.84	120.47
3	B	2341	NAP	C3N-C7N-N7N	3.24	121.47	117.77
3	O	3341	NAP	C3N-C7N-N7N	3.24	121.47	117.77
3	Q	5341	NAP	C5A-C6A-N6A	3.40	127.41	120.47
3	R	6341	NAP	C5A-C6A-N6A	3.44	127.47	120.47
3	A	1341	NAP	C3N-C7N-N7N	3.44	121.70	117.77
3	O	3341	NAP	C2N-C3N-C4N	3.50	122.25	118.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1341	NAP	2	0
2	P	4339	SO4	1	0
3	P	4341	NAP	3	0
3	Q	5341	NAP	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	338/380 (88%)	-0.47	3 (0%) 84 85	11, 25, 45, 77	0
1	B	338/380 (88%)	-0.60	3 (0%) 84 85	11, 21, 39, 81	0
1	O	338/380 (88%)	-0.46	3 (0%) 84 85	13, 27, 47, 81	0
1	P	338/380 (88%)	-0.32	8 (2%) 59 61	16, 31, 57, 89	0
1	Q	338/380 (88%)	-0.09	16 (4%) 32 34	22, 40, 62, 83	0
1	R	338/380 (88%)	-0.25	8 (2%) 59 61	19, 36, 56, 84	0
All	All	2028/2280 (88%)	-0.37	41 (2%) 65 67	11, 30, 55, 89	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	1	MET	11.1
1	B	1	MET	10.7
1	P	1	MET	8.9
1	A	1	MET	8.4
1	Q	1	MET	6.1
1	O	1	MET	5.7
1	R	127	ALA	4.0
1	R	252	GLU	3.7
1	R	338	GLY	3.6
1	Q	128	GLU	3.5
1	P	338	GLY	3.5
1	P	127	ALA	3.5
1	Q	127	ALA	3.2
1	R	126	LYS	3.1
1	A	64	GLU	3.0
1	O	338	GLY	3.0
1	Q	253	LYS	3.0
1	Q	26	ASN	3.0
1	P	64	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	Q	63	ASP	2.8
1	Q	252	GLU	2.7
1	Q	254	PRO	2.6
1	P	128	GLU	2.6
1	P	2	THR	2.6
1	Q	338	GLY	2.5
1	Q	38	SER	2.5
1	A	80	ARG	2.4
1	P	80	ARG	2.4
1	Q	101	VAL	2.4
1	R	91	ASP	2.4
1	R	143	ARG	2.4
1	B	338	GLY	2.3
1	Q	90	TRP	2.2
1	P	57	ASN	2.1
1	Q	64	GLU	2.1
1	B	140	SER	2.1
1	Q	143	ARG	2.1
1	R	128	GLU	2.1
1	O	127	ALA	2.1
1	Q	80	ARG	2.1
1	Q	140	SER	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, 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	P	4339	5/5	0.88	0.24	4.30	39,41,44,44	5
2	SO4	O	3339	5/5	0.96	0.18	2.66	33,35,36,37	5
2	SO4	B	2339	5/5	0.98	0.12	2.26	17,21,22,25	5
2	SO4	R	6339	5/5	0.96	0.16	1.01	35,36,37,40	5
2	SO4	A	1339	5/5	0.98	0.12	0.86	14,16,19,23	5
3	NAP	O	3341	48/48	0.96	0.12	0.05	19,38,56,58	0
3	NAP	Q	5341	48/48	0.95	0.14	0.02	36,43,53,58	0
3	NAP	P	4341	48/48	0.96	0.13	-0.02	25,39,48,52	0
3	NAP	R	6341	48/48	0.95	0.13	-0.21	31,43,51,56	0
3	NAP	A	1341	48/48	0.97	0.11	-0.29	16,27,42,47	0
3	NAP	B	2341	48/48	0.97	0.10	-0.41	11,25,42,45	0
2	SO4	Q	5339	5/5	0.97	0.11	-0.92	45,45,47,49	5
2	SO4	P	4340	5/5	0.98	0.11	-	28,31,34,36	5
2	SO4	Q	5340	5/5	0.98	0.13	-	27,29,34,34	5
2	SO4	O	3340	5/5	0.96	0.19	-	22,26,30,30	5
2	SO4	A	1340	5/5	0.99	0.13	-	24,27,29,31	5
2	SO4	B	2340	5/5	0.98	0.16	-	16,22,23,24	5
2	SO4	R	6340	5/5	0.97	0.17	-	25,27,33,35	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.