



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:01 PM GMT

PDB ID : 4WL0  
Title : Ligand-free structure of human platelet phosphofructokinase in an R-state, crystal form I  
Authors : Kloos, M.; Strater, N.  
Deposited on : 2014-10-05  
Resolution : 2.89 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

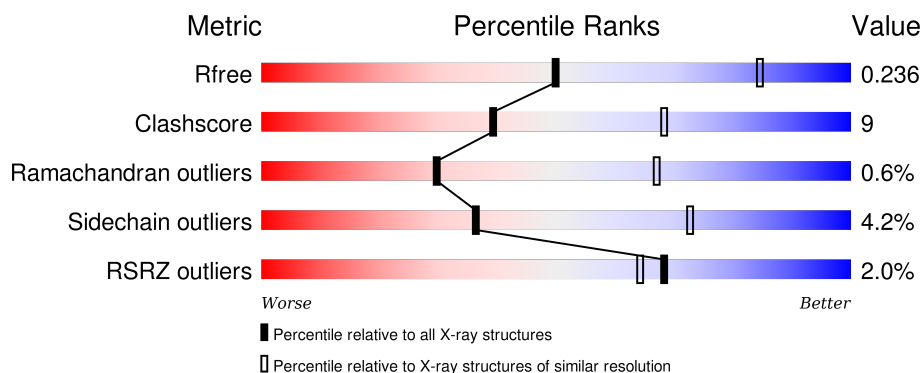
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.89 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	761	<div> <div>%</div> <div> <div></div> <div>73%</div> <div>19%</div> <div>• 6%</div> </div> </div>
1	B	761	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>• •</div> </div> </div>
1	C	761	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>19%</div> <div>• 6%</div> </div> </div>
1	D	761	<div> <div>2%</div> <div> <div></div> <div>73%</div> <div>20%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 22052 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 ATP-dependent 6-phosphofructokinase, platelet type.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	712	Total	C	N	O	S	0	0	0
			5452	3424	965	1026	37			
1	B	727	Total	C	N	O	S	0	0	0
			5554	3486	984	1046	38			
1	C	712	Total	C	N	O	S	0	0	0
			5452	3424	965	1026	37			
1	D	727	Total	C	N	O	S	0	0	0
			5554	3486	984	1046	38			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	initiating methionine	UNP Q01813
A	3	ALA	-	expression tag	UNP Q01813
A	4	SER	-	expression tag	UNP Q01813
A	5	TRP	-	expression tag	UNP Q01813
A	6	SER	-	expression tag	UNP Q01813
A	7	HIS	-	expression tag	UNP Q01813
A	8	PRO	-	expression tag	UNP Q01813
A	9	GLN	-	expression tag	UNP Q01813
A	10	PHE	-	expression tag	UNP Q01813
A	11	GLU	-	expression tag	UNP Q01813
A	12	LYS	-	expression tag	UNP Q01813
A	13	GLY	-	expression tag	UNP Q01813
A	14	ALA	-	expression tag	UNP Q01813
A	15	ASP	-	expression tag	UNP Q01813
A	16	ASP	-	expression tag	UNP Q01813
A	17	ASP	-	expression tag	UNP Q01813
A	18	ASP	-	expression tag	UNP Q01813
A	19	LYS	-	expression tag	UNP Q01813
A	20	VAL	-	expression tag	UNP Q01813
A	21	PRO	-	expression tag	UNP Q01813
A	22	ASP	-	expression tag	UNP Q01813

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Chain	Residue	Modelled	Actual	Comment	Reference
A	23	PRO	-	expression tag	UNP Q01813
A	24	THR	-	expression tag	UNP Q01813
A	25	SER	-	expression tag	UNP Q01813
B	2	MET	-	initiating methionine	UNP Q01813
B	3	ALA	-	expression tag	UNP Q01813
B	4	SER	-	expression tag	UNP Q01813
B	5	TRP	-	expression tag	UNP Q01813
B	6	SER	-	expression tag	UNP Q01813
B	7	HIS	-	expression tag	UNP Q01813
B	8	PRO	-	expression tag	UNP Q01813
B	9	GLN	-	expression tag	UNP Q01813
B	10	PHE	-	expression tag	UNP Q01813
B	11	GLU	-	expression tag	UNP Q01813
B	12	LYS	-	expression tag	UNP Q01813
B	13	GLY	-	expression tag	UNP Q01813
B	14	ALA	-	expression tag	UNP Q01813
B	15	ASP	-	expression tag	UNP Q01813
B	16	ASP	-	expression tag	UNP Q01813
B	17	ASP	-	expression tag	UNP Q01813
B	18	ASP	-	expression tag	UNP Q01813
B	19	LYS	-	expression tag	UNP Q01813
B	20	VAL	-	expression tag	UNP Q01813
B	21	PRO	-	expression tag	UNP Q01813
B	22	ASP	-	expression tag	UNP Q01813
B	23	PRO	-	expression tag	UNP Q01813
B	24	THR	-	expression tag	UNP Q01813
B	25	SER	-	expression tag	UNP Q01813
C	2	MET	-	initiating methionine	UNP Q01813
C	3	ALA	-	expression tag	UNP Q01813
C	4	SER	-	expression tag	UNP Q01813
C	5	TRP	-	expression tag	UNP Q01813
C	6	SER	-	expression tag	UNP Q01813
C	7	HIS	-	expression tag	UNP Q01813
C	8	PRO	-	expression tag	UNP Q01813
C	9	GLN	-	expression tag	UNP Q01813
C	10	PHE	-	expression tag	UNP Q01813
C	11	GLU	-	expression tag	UNP Q01813
C	12	LYS	-	expression tag	UNP Q01813
C	13	GLY	-	expression tag	UNP Q01813
C	14	ALA	-	expression tag	UNP Q01813
C	15	ASP	-	expression tag	UNP Q01813
C	16	ASP	-	expression tag	UNP Q01813

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Chain	Residue	Modelled	Actual	Comment	Reference
C	17	ASP	-	expression tag	UNP Q01813
C	18	ASP	-	expression tag	UNP Q01813
C	19	LYS	-	expression tag	UNP Q01813
C	20	VAL	-	expression tag	UNP Q01813
C	21	PRO	-	expression tag	UNP Q01813
C	22	ASP	-	expression tag	UNP Q01813
C	23	PRO	-	expression tag	UNP Q01813
C	24	THR	-	expression tag	UNP Q01813
C	25	SER	-	expression tag	UNP Q01813
D	2	MET	-	initiating methionine	UNP Q01813
D	3	ALA	-	expression tag	UNP Q01813
D	4	SER	-	expression tag	UNP Q01813
D	5	TRP	-	expression tag	UNP Q01813
D	6	SER	-	expression tag	UNP Q01813
D	7	HIS	-	expression tag	UNP Q01813
D	8	PRO	-	expression tag	UNP Q01813
D	9	GLN	-	expression tag	UNP Q01813
D	10	PHE	-	expression tag	UNP Q01813
D	11	GLU	-	expression tag	UNP Q01813
D	12	LYS	-	expression tag	UNP Q01813
D	13	GLY	-	expression tag	UNP Q01813
D	14	ALA	-	expression tag	UNP Q01813
D	15	ASP	-	expression tag	UNP Q01813
D	16	ASP	-	expression tag	UNP Q01813
D	17	ASP	-	expression tag	UNP Q01813
D	18	ASP	-	expression tag	UNP Q01813
D	19	LYS	-	expression tag	UNP Q01813
D	20	VAL	-	expression tag	UNP Q01813
D	21	PRO	-	expression tag	UNP Q01813
D	22	ASP	-	expression tag	UNP Q01813
D	23	PRO	-	expression tag	UNP Q01813
D	24	THR	-	expression tag	UNP Q01813
D	25	SER	-	expression tag	UNP Q01813

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

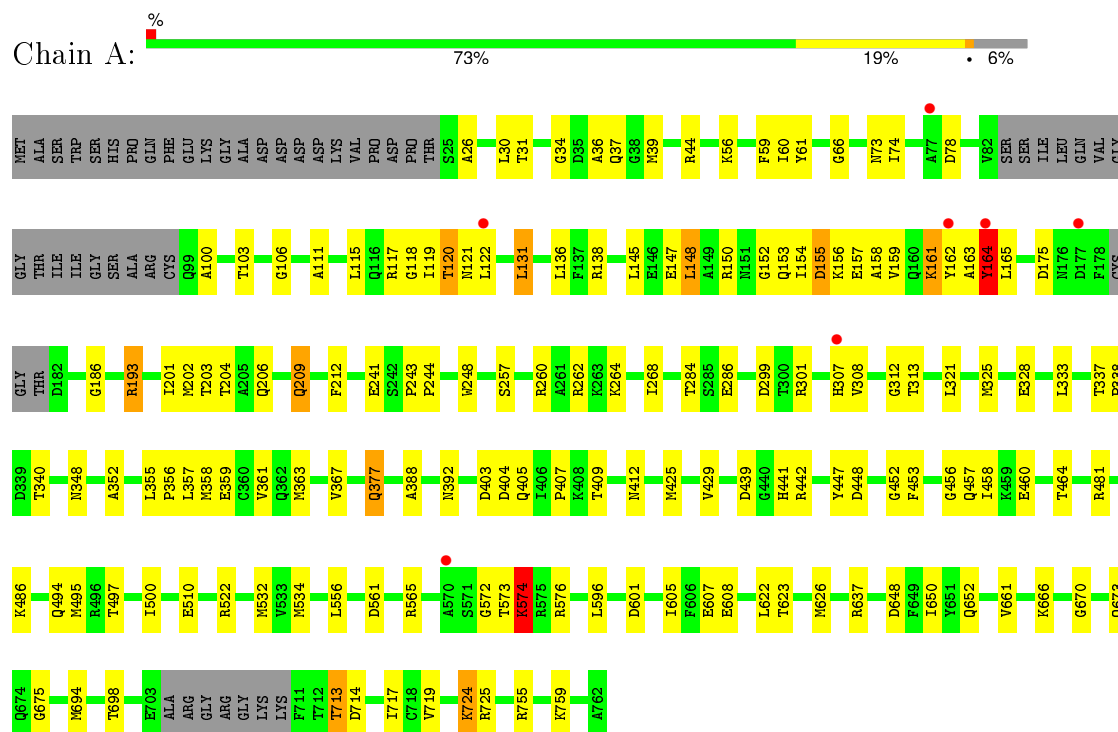


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

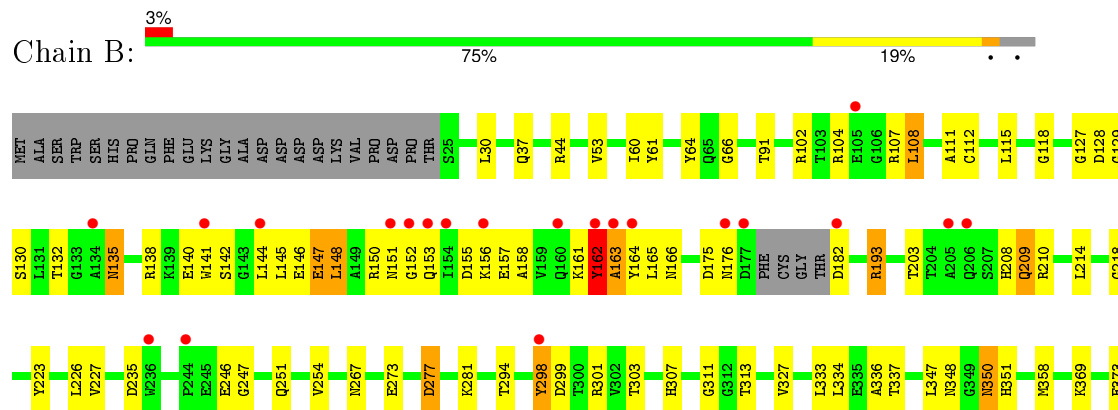
### 3 Residue-property plots

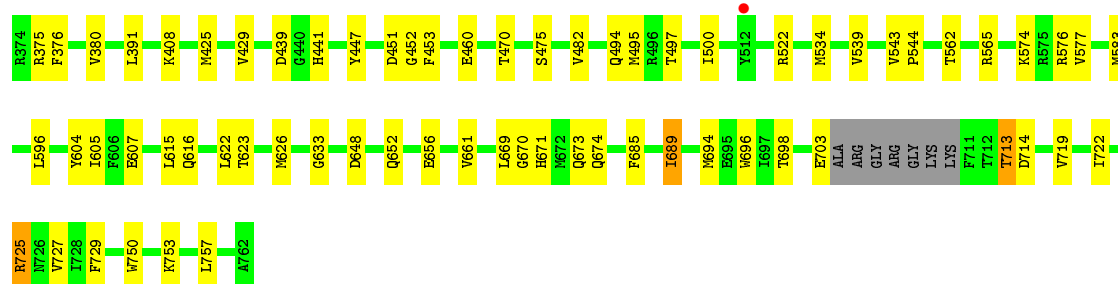
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type

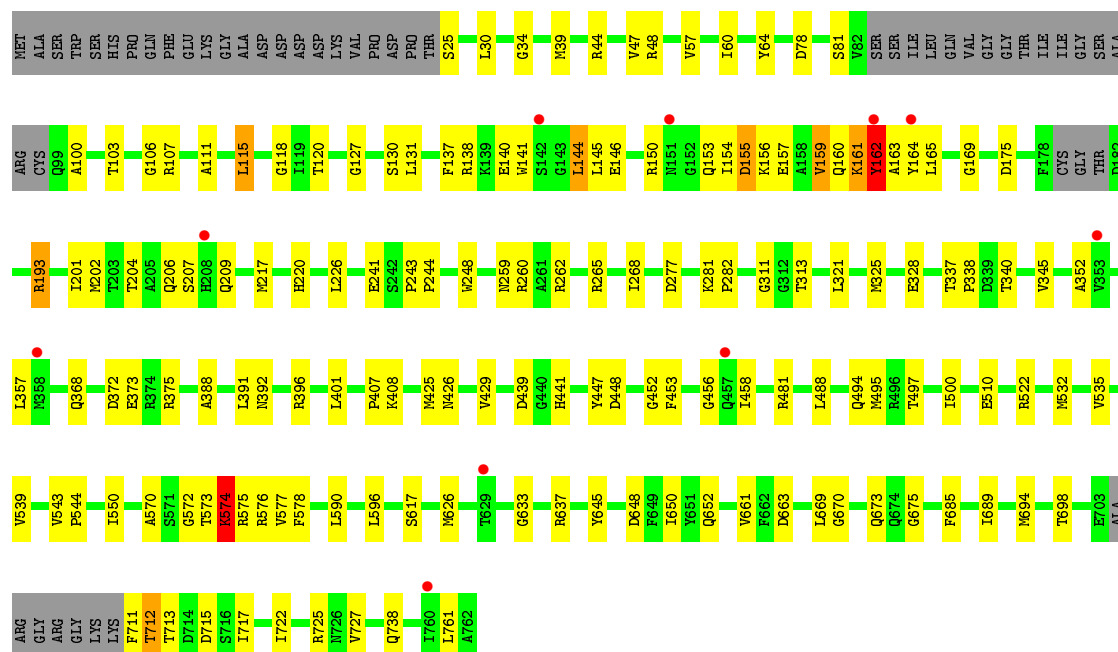
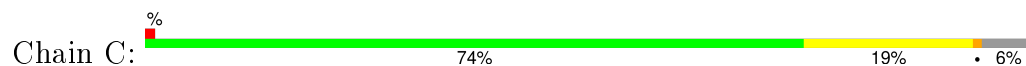


- Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type

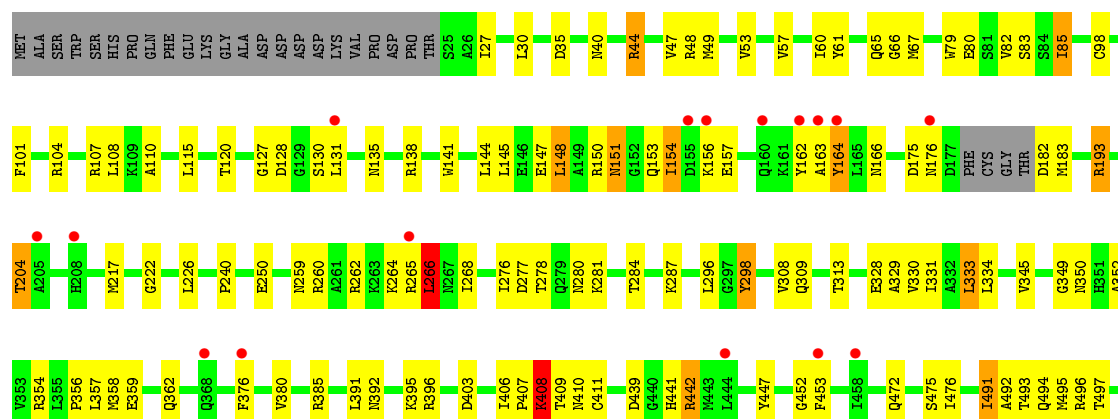
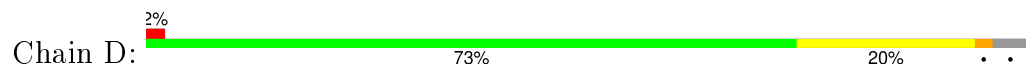




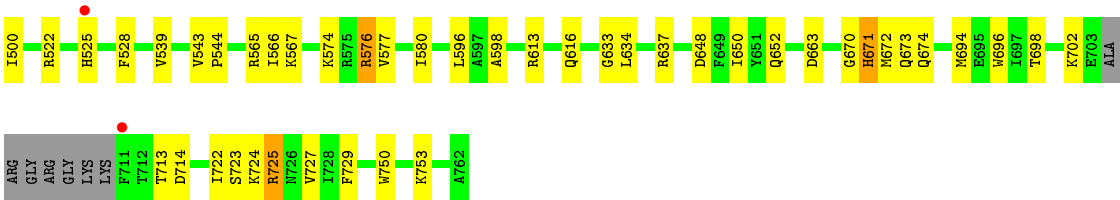
- Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type



- Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.34Å 178.06Å 133.12Å 90.00° 104.45° 90.00°	Depositor
Resolution (Å)	46.97 – 2.89 46.97 – 2.89	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.97-2.89) 99.4 (46.97-2.89)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.10 (at 2.91Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.211 , 0.236 0.210 , 0.236	Depositor DCC
$R_{free}$ test set	3980 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.7	Xtriage
Anisotropy	0.829	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 50.1	EDS
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 79810 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	22052	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.30	1/5539 (0.0%)	0.56	1/7480 (0.0%)
1	B	0.31	0/5642	0.57	1/7620 (0.0%)
1	C	0.30	0/5539	0.55	4/7480 (0.1%)
1	D	0.30	0/5642	0.55	3/7620 (0.0%)
All	All	0.30	1/22362 (0.0%)	0.56	9/30200 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	164	TYR	CD1-CE1	-5.16	1.31	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	266	LEU	CA-CB-CG	6.87	131.11	115.30
1	D	148	LEU	CA-CB-CG	6.82	130.99	115.30
1	D	266	LEU	CB-CG-CD1	5.90	121.03	111.00
1	A	148	LEU	CA-CB-CG	5.82	128.69	115.30
1	C	488	LEU	CB-CG-CD2	-5.77	101.19	111.00
1	C	144	LEU	CA-CB-CG	5.62	128.22	115.30
1	B	725	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	C	115	LEU	CB-CG-CD2	-5.28	102.02	111.00
1	C	161	LYS	N-CA-C	5.04	124.61	111.00

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	5452	0	5465	98	0
1	B	5554	0	5579	99	0
1	C	5452	0	5465	109	0
1	D	5554	0	5579	105	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	1	0
All	All	22052	0	22088	394	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 9.

All (394) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:396:ARG:NH2	1:C:439:ASP:OD1	2.05	0.90
1:D:40:ASN:HB3	1:D:85:ILE:HG23	1.59	0.85
1:B:713:THR:OG1	1:B:714:ASP:N	2.10	0.84
1:D:349:GLY:HA3	1:D:725:ARG:HB3	1.60	0.83
1:D:296:LEU:HB3	1:D:298:TYR:CE2	2.15	0.81
1:A:209:GLN:NE2	1:A:264:LYS:O	2.13	0.81
1:C:669:LEU:HD23	1:D:672:MET:HE1	1.63	0.80
1:C:115:LEU:HD21	1:C:164:TYR:OH	1.82	0.80
1:A:157:GLU:O	1:A:161:LYS:HB2	1.82	0.79
1:C:209:GLN:OE1	1:C:260:ARG:NH1	2.18	0.77
1:A:348:ASN:OD1	1:A:725:ARG:NH2	2.19	0.75
1:B:107:ARG:NH1	1:B:140:GLU:OE1	2.19	0.74
1:D:296:LEU:HB3	1:D:298:TYR:HE2	1.53	0.74
1:B:118:GLY:HA2	1:B:161:LYS:HE2	1.70	0.73
1:A:713:THR:OG1	1:A:714:ASP:N	2.21	0.72
1:D:138:ARG:HH12	1:D:166:ASN:HA	1.55	0.72
1:B:348:ASN:HB3	1:B:725:ARG:NH2	2.05	0.72
1:A:103:THR:HG23	1:A:106:GLY:H	1.54	0.72
1:D:259:ASN:OD1	1:D:262:ARG:NH2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ARG:NH2	1:C:313:THR:O	2.23	0.71
1:B:147:GLU:OE1	1:B:153:GLN:HG2	1.92	0.70
1:C:259:ASN:OD1	1:C:262:ARG:NH2	2.21	0.70
1:A:388:ALA:O	1:A:392:ASN:ND2	2.25	0.69
1:C:388:ALA:O	1:C:392:ASN:ND2	2.26	0.69
1:C:368:GLN:NE2	1:C:372:ASP:OD1	2.26	0.68
1:B:218:GLY:H	1:B:273:GLU:HG2	1.58	0.67
1:A:131:LEU:HD13	1:A:357:LEU:HD11	1.75	0.66
1:B:670:GLY:O	1:B:673:GLN:HG2	1.95	0.66
1:A:522:ARG:NH1	1:A:713:THR:O	2.29	0.66
1:B:623:THR:HG23	1:B:661:VAL:HG11	1.77	0.66
1:D:193:ARG:NH2	1:D:313:THR:O	2.28	0.66
1:D:522:ARG:NH1	1:D:713:THR:O	2.29	0.66
1:A:494:GLN:HA	1:A:497:THR:HG22	1.78	0.66
1:D:670:GLY:O	1:D:673:GLN:HG2	1.96	0.66
1:C:535:VAL:HB	1:C:689:ILE:HD12	1.79	0.65
1:D:276:ILE:HG23	1:D:280:ASN:HA	1.78	0.65
1:C:78:ASP:OD1	1:C:81:SER:OG	2.15	0.64
1:A:138:ARG:HA	1:A:165:LEU:HD23	1.80	0.64
1:B:351:HIS:N	1:B:725:ARG:HH12	1.95	0.63
1:C:107:ARG:NH1	1:C:140:GLU:OE1	2.31	0.63
1:D:115:LEU:HD11	1:D:144:LEU:HD21	1.79	0.63
1:C:550:ILE:HD11	1:C:689:ILE:HD11	1.79	0.63
1:A:155:ASP:OD1	1:A:155:ASP:N	2.30	0.63
1:A:648:ASP:O	1:A:652:GLN:HG3	1.99	0.62
1:B:348:ASN:HB3	1:B:725:ARG:HH21	1.63	0.62
1:C:373:GLU:OE1	1:C:375:ARG:NH1	2.31	0.62
1:B:648:ASP:O	1:B:652:GLN:HG3	2.00	0.62
1:A:299:ASP:OD1	1:A:301:ARG:NH1	2.33	0.62
1:D:410:ASN:HA	1:D:442:ARG:HH12	1.65	0.62
1:D:182:ASP:OD1	1:D:183:MET:N	2.33	0.61
1:C:131:LEU:HD23	1:C:357:LEU:HD13	1.82	0.61
1:D:648:ASP:O	1:D:652:GLN:HG3	2.00	0.61
1:C:648:ASP:O	1:C:652:GLN:HG3	2.01	0.61
1:C:144:LEU:HD21	1:C:164:TYR:HE2	1.65	0.61
1:B:441:HIS:NE2	1:B:698:THR:HG22	2.15	0.61
1:C:30:LEU:HB3	1:C:60:ILE:HB	1.84	0.60
1:D:120:THR:HB	1:D:164:TYR:O	2.02	0.60
1:C:663:ASP:N	1:C:663:ASP:OD1	2.34	0.60
1:A:74:ILE:HD11	1:A:117:ARG:NE	2.17	0.60
1:B:210:ARG:NH1	1:B:299:ASP:OD2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:494:GLN:HA	1:B:497:THR:HG22	1.83	0.59
1:D:53:VAL:HG21	1:D:334:LEU:HD11	1.83	0.59
1:D:539:VAL:HG11	1:D:674:GLN:HB2	1.84	0.59
1:C:146:GLU:O	1:C:150:ARG:HG2	2.02	0.59
1:C:157:GLU:N	1:C:157:GLU:OE1	2.35	0.59
1:B:144:LEU:HD21	1:B:158:ALA:HA	1.83	0.59
1:A:193:ARG:NH2	1:A:313:THR:O	2.35	0.59
1:A:328:GLU:HG2	1:A:352:ALA:HB1	1.86	0.58
1:B:750:TRP:O	1:B:753:LYS:HG2	2.03	0.58
1:B:162:TYR:C	1:B:164:TYR:H	2.07	0.58
1:B:166:ASN:ND2	1:B:333:LEU:O	2.36	0.58
1:A:441:HIS:NE2	1:A:698:THR:HG22	2.19	0.58
1:C:48:ARG:NH1	1:C:761:LEU:O	2.36	0.58
1:D:359:GLU:OE1	1:D:359:GLU:N	2.37	0.57
1:C:137:PHE:CZ	1:C:141:TRP:HZ3	2.23	0.57
1:C:154:ILE:HB	1:C:157:GLU:OE1	2.04	0.57
1:D:260:ARG:HD3	1:D:298:TYR:OH	2.05	0.57
1:D:217:MET:HG3	1:D:309:GLN:NE2	2.20	0.56
1:A:724:LYS:HG3	1:A:725:ARG:N	2.21	0.56
1:C:156:LYS:O	1:C:160:GLN:HB2	2.06	0.56
1:C:328:GLU:HG2	1:C:352:ALA:HB1	1.86	0.56
1:D:27:ILE:HG12	1:D:333:LEU:HD23	1.87	0.56
1:D:98:CYS:SG	1:D:101:PHE:HB2	2.46	0.55
1:C:137:PHE:CE2	1:C:141:TRP:HZ3	2.23	0.55
1:C:539:VAL:O	1:C:590:LEU:HD11	2.07	0.55
1:C:570:ALA:HB1	1:C:573:THR:OG1	2.05	0.55
1:C:439:ASP:OD2	1:C:698:THR:HG21	2.07	0.55
1:A:573:THR:O	1:A:574:LYS:HG2	2.06	0.55
1:C:522:ARG:NH1	1:C:713:THR:O	2.40	0.55
1:D:410:ASN:HA	1:D:442:ARG:NH1	2.22	0.55
1:B:148:LEU:HD11	1:B:158:ALA:HB2	1.89	0.55
1:D:493:THR:O	1:D:496:ARG:HG2	2.07	0.55
1:D:441:HIS:NE2	1:D:698:THR:HG22	2.22	0.54
1:A:637:ARG:HD2	1:A:650:ILE:HD12	1.89	0.54
1:B:150:ARG:O	1:B:152:GLY:N	2.40	0.54
1:C:441:HIS:NE2	1:C:698:THR:HG22	2.22	0.54
1:B:142:SER:O	1:B:145:LEU:HG	2.06	0.54
1:B:369:LYS:O	1:B:373:GLU:HG2	2.08	0.54
1:A:675:GLY:HA2	1:B:565:ARG:NH1	2.22	0.54
1:B:102:ARG:C	1:B:107:ARG:HH21	2.10	0.54
1:B:155:ASP:C	1:B:157:GLU:H	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:HIS:CE1	1:B:301:ARG:HB3	2.43	0.54
1:B:193:ARG:NH2	1:B:313:THR:O	2.40	0.54
1:C:207:SER:HB2	1:D:35:ASP:HB2	1.89	0.54
1:C:244:PRO:HB2	1:C:248:TRP:CG	2.43	0.54
1:C:131:LEU:HD22	1:C:169:GLY:HA3	1.89	0.54
1:B:251:GLN:O	1:B:254:VAL:HG12	2.07	0.54
1:A:34:GLY:HA3	1:A:39:MET:CE	2.38	0.54
1:C:141:TRP:CZ2	1:C:164:TYR:CZ	2.95	0.54
1:A:159:VAL:HA	1:A:162:TYR:CE2	2.43	0.54
1:B:135:ASN:O	1:B:138:ARG:HB3	2.08	0.54
1:B:351:HIS:H	1:B:725:ARG:HH12	1.55	0.53
1:D:226:LEU:HD11	1:D:391:LEU:HA	1.90	0.53
1:A:605:ILE:HD12	1:A:607:GLU:HB2	1.89	0.53
1:A:158:ALA:O	1:A:162:TYR:HD2	1.89	0.53
1:C:141:TRP:NE1	1:C:164:TYR:CZ	2.77	0.53
1:D:392:ASN:OD1	1:D:396:ARG:NH1	2.37	0.53
1:D:724:LYS:O	1:D:725:ARG:HG2	2.09	0.53
1:B:53:VAL:HG21	1:B:334:LEU:HD11	1.90	0.53
1:B:685:PHE:HE2	1:B:689:ILE:HG13	1.73	0.53
1:C:494:GLN:HA	1:C:497:THR:HG22	1.90	0.53
1:D:104:ARG:O	1:D:108:LEU:HD13	2.09	0.53
1:B:141:TRP:CE3	1:B:165:LEU:HD22	2.44	0.52
1:C:685:PHE:O	1:C:689:ILE:HG12	2.09	0.52
1:A:284:THR:HB	1:A:286:GLU:OE1	2.09	0.52
1:C:481:ARG:NH1	1:C:510:GLU:OE2	2.42	0.52
1:D:150:ARG:O	1:D:150:ARG:NH1	2.42	0.52
1:A:193:ARG:HG3	1:A:308:VAL:HG12	1.92	0.52
1:D:577:VAL:HG22	1:D:633:GLY:HA3	1.91	0.52
1:C:141:TRP:HZ2	1:C:164:TYR:CZ	2.28	0.52
1:C:141:TRP:HZ2	1:C:164:TYR:HH	1.54	0.52
1:C:155:ASP:OD1	1:C:155:ASP:N	2.42	0.52
1:A:495:MET:HG2	1:A:500:ILE:HD12	1.91	0.52
1:D:264:LYS:NZ	2:D:801:PO4:O2	2.31	0.52
1:C:100:ALA:O	1:C:103:THR:HG22	2.10	0.52
1:C:637:ARG:HD2	1:C:650:ILE:HD12	1.91	0.52
1:B:522:ARG:NH1	1:B:713:THR:O	2.42	0.52
1:C:111:ALA:O	1:C:115:LEU:HG	2.10	0.51
1:D:30:LEU:HB3	1:D:60:ILE:HB	1.91	0.51
1:A:61:TYR:O	1:A:66:GLY:HA3	2.10	0.51
1:D:495:MET:HG2	1:D:500:ILE:HD12	1.92	0.51
1:D:153:GLN:OE1	1:D:153:GLN:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:578:PHE:HE2	1:D:671:HIS:CE1	2.27	0.51
1:D:392:ASN:O	1:D:395:LYS:HG2	2.11	0.51
1:D:494:GLN:HA	1:D:497:THR:HG22	1.93	0.51
1:C:447:TYR:O	1:C:452:GLY:HA3	2.10	0.51
1:B:351:HIS:HB3	1:B:725:ARG:NH1	2.26	0.51
1:D:135:ASN:HB2	1:D:357:LEU:HD23	1.93	0.51
1:A:164:TYR:HD1	1:A:164:TYR:C	2.14	0.51
1:C:575:ARG:NH1	1:C:626:MET:HB3	2.26	0.51
1:A:145:LEU:HA	1:A:148:LEU:HG	1.92	0.51
1:B:115:LEU:HD11	1:B:144:LEU:HD12	1.94	0.50
1:A:145:LEU:HD23	1:A:148:LEU:HD21	1.93	0.50
1:B:694:MET:O	1:B:698:THR:HG23	2.11	0.50
1:C:448:ASP:OD1	1:D:574:LYS:HD2	2.12	0.50
1:B:277:ASP:N	1:B:281:LYS:O	2.44	0.50
1:D:567:LYS:NZ	1:D:598:ALA:O	2.28	0.50
1:B:30:LEU:HB3	1:B:60:ILE:HB	1.94	0.50
1:D:154:ILE:HG12	1:D:157:GLU:OE1	2.11	0.50
1:A:623:THR:HG23	1:A:661:VAL:HG21	1.93	0.50
1:A:30:LEU:HB3	1:A:60:ILE:HB	1.94	0.50
1:D:566:ILE:HG21	1:D:580:ILE:HD11	1.92	0.50
1:D:115:LEU:HD11	1:D:144:LEU:CD2	2.42	0.50
1:C:713:THR:OG1	1:C:715:ASP:OD1	2.26	0.50
1:A:358:MET:HA	1:A:361:VAL:HG22	1.94	0.50
1:B:214:LEU:HD22	1:B:303:THR:HB	1.93	0.50
1:D:145:LEU:O	1:D:148:LEU:HG	2.12	0.49
1:C:670:GLY:O	1:C:673:GLN:HG3	2.12	0.49
1:C:575:ARG:HH12	1:C:661:VAL:HG13	1.77	0.49
1:B:162:TYR:O	1:B:164:TYR:N	2.46	0.49
1:C:575:ARG:HD3	1:C:661:VAL:O	2.13	0.49
1:B:347:LEU:HG	1:B:350:ASN:H	1.78	0.49
1:A:670:GLY:O	1:A:673:GLN:HG3	2.11	0.49
1:C:202:MET:HG2	1:C:268:ILE:HD11	1.93	0.49
1:C:141:TRP:HZ2	1:C:164:TYR:CE1	2.31	0.49
1:D:409:THR:O	1:D:442:ARG:NH1	2.46	0.49
1:B:104:ARG:NH2	1:B:146:GLU:OE1	2.44	0.49
1:B:376:PHE:O	1:B:380:VAL:HG23	2.12	0.49
1:D:472:GLN:HG2	1:D:476:ILE:HD11	1.95	0.49
1:A:572:GLY:HA3	1:B:475:SER:O	2.13	0.49
1:D:576:ARG:NH1	1:D:663:ASP:OD2	2.45	0.49
1:A:244:PRO:HB2	1:A:248:TRP:CG	2.48	0.49
1:C:694:MET:O	1:C:698:THR:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:403:ASP:O	1:D:408:LYS:NZ	2.32	0.48
1:A:206:GLN:OE1	1:A:206:GLN:N	2.46	0.48
1:A:404:ASP:OD1	1:A:405:GLN:HG3	2.13	0.48
1:B:145:LEU:HD12	1:B:146:GLU:N	2.27	0.48
1:D:127:GLY:O	1:D:130:SER:OG	2.32	0.48
1:D:104:ARG:HG2	1:D:107:ARG:NH1	2.28	0.48
1:C:144:LEU:HD21	1:C:164:TYR:CE2	2.47	0.48
1:D:406:ILE:HB	1:D:408:LYS:HZ2	1.79	0.48
1:A:202:MET:HG2	1:A:268:ILE:HD11	1.95	0.48
1:C:204:THR:C	1:C:206:GLN:H	2.17	0.48
1:C:131:LEU:HG	1:C:357:LEU:HD22	1.95	0.48
1:B:439:ASP:OD2	1:B:698:THR:HG21	2.14	0.48
1:D:356:PRO:HB2	1:D:359:GLU:OE1	2.13	0.48
1:A:161:LYS:HA	1:A:164:TYR:CE2	2.48	0.48
1:B:111:ALA:O	1:B:115:LEU:HG	2.14	0.48
1:A:59:PHE:O	1:A:74:ILE:HA	2.14	0.48
1:A:164:TYR:C	1:A:164:TYR:CD1	2.87	0.48
1:A:622:LEU:O	1:A:626:MET:HG2	2.14	0.48
1:A:442:ARG:NH2	1:A:460:GLU:HB3	2.29	0.47
1:B:656:GLU:HG2	1:C:645:TYR:CZ	2.50	0.47
1:D:260:ARG:HD3	1:D:298:TYR:CZ	2.49	0.47
1:C:161:LYS:O	1:C:164:TYR:HD2	1.98	0.47
1:A:147:GLU:HB2	1:A:153:GLN:HE21	1.78	0.47
1:C:711:PHE:O	1:C:712:THR:HG23	2.15	0.47
1:A:37:GLN:HE22	1:B:203:THR:HG22	1.79	0.47
1:B:577:VAL:HG22	1:B:633:GLY:HA3	1.97	0.47
1:B:685:PHE:CE2	1:B:689:ILE:HG13	2.49	0.47
1:A:363:MET:O	1:A:367:VAL:HG23	2.15	0.47
1:C:241:GLU:O	1:C:243:PRO:HD3	2.14	0.47
1:D:525:HIS:HB2	1:D:528:PHE:CE2	2.50	0.47
1:D:447:TYR:O	1:D:452:GLY:HA3	2.14	0.47
1:C:675:GLY:HA2	1:D:565:ARG:HH11	1.78	0.47
1:C:141:TRP:O	1:C:144:LEU:HD13	2.15	0.47
1:B:145:LEU:HB3	1:B:162:TYR:OH	2.15	0.47
1:A:439:ASP:OD2	1:A:698:THR:HG21	2.15	0.47
1:B:61:TYR:O	1:B:66:GLY:HA3	2.14	0.46
1:D:284:THR:H	1:D:287:LYS:HD2	1.80	0.46
1:B:193:ARG:HD3	1:B:193:ARG:HA	1.64	0.46
1:D:406:ILE:HB	1:D:408:LYS:NZ	2.29	0.46
1:D:222:GLY:HA3	1:D:240:PRO:HD2	1.97	0.46
1:A:34:GLY:HA3	1:A:39:MET:HE1	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:ASN:ND2	1:B:336:ALA:HB3	2.30	0.46
1:B:129:GLY:HA2	1:B:132:THR:HG23	1.97	0.46
1:D:328:GLU:HG2	1:D:352:ALA:HB1	1.96	0.46
1:C:675:GLY:HA2	1:D:565:ARG:NH1	2.31	0.46
1:C:34:GLY:HA3	1:C:39:MET:CE	2.46	0.46
1:B:156:LYS:HE2	1:B:156:LYS:HB2	1.59	0.46
1:B:209:GLN:OE1	1:B:298:TYR:OH	2.32	0.46
1:A:601:ASP:O	1:A:759:LYS:NZ	2.33	0.46
1:D:580:ILE:HD12	1:D:634:LEU:HD11	1.98	0.46
1:A:456:GLY:HA2	1:A:458:ILE:HD12	1.97	0.46
1:A:448:ASP:OD1	1:B:574:LYS:HD2	2.15	0.46
1:D:409:THR:OG1	1:D:441:HIS:ND1	2.49	0.46
1:D:694:MET:O	1:D:698:THR:HG23	2.16	0.46
1:A:147:GLU:HB2	1:A:153:GLN:NE2	2.31	0.45
1:D:80:GLU:O	1:D:83:SER:OG	2.31	0.45
1:C:572:GLY:HA3	1:D:475:SER:O	2.16	0.45
1:D:439:ASP:OD2	1:D:698:THR:HG21	2.16	0.45
1:B:108:LEU:HD13	1:B:150:ARG:HH21	1.82	0.45
1:C:103:THR:HG23	1:C:106:GLY:H	1.81	0.45
1:A:111:ALA:O	1:A:115:LEU:HG	2.16	0.45
1:B:226:LEU:HD11	1:B:391:LEU:HA	1.99	0.45
1:C:78:ASP:N	1:C:81:SER:OG	2.39	0.45
1:A:481:ARG:NH1	1:A:510:GLU:OE2	2.49	0.45
1:D:296:LEU:HB3	1:D:298:TYR:CD2	2.50	0.45
1:B:162:TYR:HB3	1:B:163:ALA:H	1.27	0.45
1:C:277:ASP:OD2	1:C:281:LYS:HB3	2.16	0.45
1:C:337:THR:H	1:C:340:THR:HB	1.82	0.45
1:B:451:ASP:HB2	1:B:482:VAL:HG11	1.98	0.45
1:D:193:ARG:HD3	1:D:193:ARG:HA	1.68	0.45
1:B:622:LEU:O	1:B:626:MET:HG2	2.16	0.45
1:B:144:LEU:C	1:B:144:LEU:HD23	2.37	0.45
1:C:425:MET:O	1:C:429:VAL:HG23	2.17	0.45
1:A:561:ASP:HB3	1:A:565:ARG:HH12	1.82	0.45
1:A:648:ASP:OD1	1:A:666:LYS:NZ	2.26	0.45
1:D:67:MET:HG2	1:D:110:ALA:HB1	1.99	0.45
1:C:47:VAL:HA	1:C:57:VAL:HG11	1.98	0.45
1:A:209:GLN:HG2	1:A:260:ARG:NH2	2.31	0.44
1:D:138:ARG:NH1	1:D:166:ASN:HA	2.28	0.44
1:B:583:MET:HG3	1:B:673:GLN:NE2	2.33	0.44
1:C:34:GLY:HA3	1:C:39:MET:HE1	1.99	0.44
1:C:281:LYS:HG3	1:C:282:PRO:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:577:VAL:HG22	1:C:633:GLY:HA3	1.99	0.44
1:C:669:LEU:HB2	1:C:673:GLN:NE2	2.33	0.44
1:D:264:LYS:HE2	1:D:266:LEU:HD12	2.00	0.44
1:A:425:MET:O	1:A:429:VAL:HG23	2.17	0.44
1:B:605:ILE:HD12	1:B:607:GLU:HB2	1.99	0.44
1:A:120:THR:HB	1:A:164:TYR:CE1	2.52	0.44
1:C:163:ALA:HB1	1:C:338:PRO:HB3	2.00	0.44
1:A:156:LYS:N	1:A:156:LYS:HD2	2.31	0.44
1:C:144:LEU:HD11	1:C:164:TYR:HH	1.83	0.44
1:D:491:ILE:HG13	1:D:492:ALA:N	2.32	0.44
1:B:246:GLU:HA	1:B:247:GLY:HA2	1.66	0.44
1:A:26:ALA:HB3	1:A:119:ILE:HA	1.98	0.44
1:A:122:LEU:HA	1:A:122:LEU:HD23	1.81	0.44
1:C:64:TYR:OH	1:C:130:SER:O	2.30	0.44
1:D:713:THR:OG1	1:D:714:ASP:N	2.50	0.44
1:C:590:LEU:H	1:C:590:LEU:HD12	1.82	0.44
1:D:141:TRP:HD1	1:D:163:ALA:H	1.65	0.44
1:B:64:TYR:OH	1:B:130:SER:O	2.19	0.44
1:C:495:MET:HA	1:C:500:ILE:HD12	1.99	0.44
1:C:118:GLY:O	1:C:120:THR:HG23	2.18	0.44
1:C:217:MET:O	1:C:217:MET:HG3	2.17	0.44
1:C:141:TRP:CE3	1:C:165:LEU:HD22	2.53	0.43
1:C:141:TRP:CZ2	1:C:164:TYR:CE1	3.05	0.43
1:A:100:ALA:O	1:A:103:THR:HG22	2.17	0.43
1:C:311:GLY:HA2	1:D:204:THR:HG23	2.00	0.43
1:C:574:LYS:HB3	1:C:574:LYS:HE3	1.60	0.43
1:B:583:MET:HE2	1:B:583:MET:HB2	1.86	0.43
1:A:694:MET:O	1:A:698:THR:HG23	2.18	0.43
1:B:277:ASP:HB2	1:B:281:LYS:HB2	2.00	0.43
1:A:56:LYS:HD2	1:A:56:LYS:HA	1.84	0.43
1:D:566:ILE:HD13	1:D:580:ILE:CD1	2.48	0.43
1:B:425:MET:O	1:B:429:VAL:HG23	2.18	0.43
1:A:262:ARG:HD2	1:A:464:THR:OG1	2.19	0.43
1:A:321:LEU:O	1:A:325:MET:HG2	2.18	0.43
1:D:750:TRP:O	1:D:753:LYS:HG2	2.17	0.43
1:A:725:ARG:HG2	1:A:725:ARG:O	2.18	0.43
1:A:356:PRO:HG2	1:A:359:GLU:CD	2.39	0.43
1:A:131:LEU:H	1:A:131:LEU:HG	1.45	0.43
1:D:277:ASP:N	1:D:281:LYS:O	2.47	0.43
1:D:47:VAL:HA	1:D:57:VAL:HG11	2.01	0.43
1:B:102:ARG:O	1:B:107:ARG:NH2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ARG:HG3	1:A:165:LEU:O	2.17	0.43
1:B:135:ASN:HD22	1:B:135:ASN:C	2.21	0.43
1:D:329:ALA:HA	1:D:345:VAL:HG11	2.00	0.43
1:A:201:ILE:O	1:A:204:THR:HG22	2.19	0.43
1:B:583:MET:SD	1:B:671:HIS:HA	2.59	0.43
1:D:543:VAL:HA	1:D:544:PRO:HD3	1.91	0.43
1:D:150:ARG:NH1	1:D:151:ASN:OD1	2.52	0.42
1:D:48:ARG:HD3	1:D:79:TRP:CZ2	2.54	0.42
1:B:543:VAL:HA	1:B:544:PRO:HD3	1.92	0.42
1:A:121:ASN:HB3	1:A:333:LEU:HD22	2.01	0.42
1:D:722:ILE:HG12	1:D:727:VAL:HG12	2.00	0.42
1:A:150:ARG:NH1	1:A:152:GLY:HA3	2.33	0.42
1:D:49:MET:HB3	1:D:330:VAL:HG21	2.02	0.42
1:D:44:ARG:HA	1:D:82:VAL:HG11	2.00	0.42
1:C:159:VAL:C	1:C:161:LYS:N	2.69	0.42
1:C:226:LEU:HD11	1:C:391:LEU:HA	2.01	0.42
1:A:608:GLU:CD	1:A:755:ARG:HH21	2.23	0.42
1:A:403:ASP:OD1	1:A:404:ASP:N	2.52	0.42
1:C:201:ILE:O	1:C:204:THR:HG22	2.20	0.42
1:A:447:TYR:O	1:A:452:GLY:HA3	2.20	0.42
1:B:539:VAL:HG11	1:B:674:GLN:HB2	2.01	0.42
1:B:128:ASP:OD1	1:B:128:ASP:N	2.51	0.42
1:C:138:ARG:HA	1:C:165:LEU:HD23	2.02	0.42
1:A:118:GLY:O	1:A:120:THR:HG22	2.20	0.42
1:B:164:TYR:N	1:B:164:TYR:CD2	2.87	0.42
1:D:406:ILE:HA	1:D:407:PRO:HD2	1.88	0.42
1:B:37:GLN:NE2	1:B:311:GLY:O	2.51	0.42
1:A:153:GLN:HB2	1:A:157:GLU:OE1	2.20	0.42
1:C:209:GLN:HA	1:C:265:ARG:O	2.20	0.42
1:D:135:ASN:ND2	1:D:358:MET:SD	2.93	0.42
1:A:312:GLY:O	1:B:203:THR:HG21	2.19	0.42
1:A:163:ALA:O	1:A:338:PRO:HB3	2.20	0.42
1:C:193:ARG:HA	1:C:193:ARG:HD3	1.58	0.41
1:A:241:GLU:O	1:A:243:PRO:HD3	2.19	0.41
1:B:327:VAL:HG21	1:B:757:LEU:HD22	2.02	0.41
1:C:120:THR:HB	1:C:164:TYR:HD1	1.84	0.41
1:A:495:MET:HA	1:A:500:ILE:HD12	2.01	0.41
1:B:235:ASP:OD2	1:B:267:ASN:HA	2.21	0.41
1:A:556:LEU:HD23	1:A:556:LEU:HA	1.91	0.41
1:D:144:LEU:HA	1:D:147:GLU:OE1	2.19	0.41
1:C:127:GLY:O	1:C:130:SER:OG	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:TRP:HE1	1:D:162:TYR:HA	1.86	0.41
1:A:36:ALA:HB1	1:A:186:GLY:HA3	2.02	0.41
1:A:212:PHE:HZ	1:B:307:HIS:ND1	2.17	0.41
1:C:543:VAL:HA	1:C:544:PRO:HD3	1.94	0.41
1:C:162:TYR:O	1:C:163:ALA:HB3	2.20	0.41
1:A:532:MET:O	1:A:717:ILE:HA	2.21	0.41
1:B:495:MET:HA	1:B:500:ILE:HD12	2.03	0.41
1:C:209:GLN:HG2	1:C:265:ARG:HA	2.03	0.41
1:D:396:ARG:HG3	1:D:396:ARG:HH11	1.85	0.41
1:A:447:TYR:HB2	1:A:457:GLN:HG2	2.03	0.41
1:A:534:MET:HG2	1:A:719:VAL:HG22	2.02	0.41
1:B:534:MET:HG2	1:B:719:VAL:HG22	2.02	0.41
1:D:331:ILE:HG22	1:D:354:ARG:NH2	2.36	0.41
1:D:696:TRP:HB2	1:D:729:PHE:CZ	2.56	0.41
1:D:65:GLN:HG3	1:D:98:CYS:HA	2.02	0.41
1:C:120:THR:HG22	1:C:164:TYR:CD1	2.55	0.41
1:C:44:ARG:HH21	1:C:48:ARG:HH12	1.69	0.41
1:A:412:ASN:OD1	1:A:442:ARG:HB3	2.21	0.41
1:B:604:TYR:CZ	1:B:615:LEU:HD23	2.56	0.41
1:B:447:TYR:O	1:B:452:GLY:HA3	2.21	0.41
1:B:175:ASP:OD1	1:B:176:ASN:N	2.53	0.41
1:D:376:PHE:O	1:D:380:VAL:HG23	2.21	0.41
1:C:165:LEU:HA	1:C:165:LEU:HD12	1.76	0.41
1:B:182:ASP:OD1	1:B:348:ASN:HA	2.21	0.41
1:A:61:TYR:N	1:A:73:ASN:O	2.48	0.41
1:C:722:ILE:HG12	1:C:727:VAL:HG12	2.03	0.41
1:B:375:ARG:HD2	1:B:375:ARG:HH11	1.73	0.41
1:C:321:LEU:O	1:C:325:MET:HG2	2.21	0.41
1:C:456:GLY:HA2	1:C:458:ILE:HD12	2.03	0.41
1:B:223:TYR:CZ	1:B:227:VAL:HG21	2.55	0.41
1:A:675:GLY:HA2	1:B:565:ARG:HH11	1.85	0.41
1:A:377:GLN:HG2	1:A:377:GLN:H	1.61	0.41
1:D:411:CYS:O	1:D:442:ARG:HG2	2.21	0.40
1:B:165:LEU:HD12	1:B:165:LEU:HA	1.94	0.40
1:D:637:ARG:HD2	1:D:650:ILE:HD12	2.03	0.40
1:A:136:LEU:HA	1:A:136:LEU:HD23	1.86	0.40
1:C:144:LEU:HD11	1:C:164:TYR:OH	2.20	0.40
1:D:495:MET:HA	1:D:500:ILE:HD12	2.03	0.40
1:B:722:ILE:HG12	1:B:727:VAL:HG12	2.04	0.40
1:C:153:GLN:N	1:C:153:GLN:OE1	2.55	0.40
1:D:702:LYS:HD2	1:D:702:LYS:HA	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:613:ARG:HG2	1:D:613:ARG:H	1.67	0.40
1:D:61:TYR:O	1:D:66:GLY:HA3	2.21	0.40
1:B:127:GLY:O	1:B:130:SER:OG	2.39	0.40
1:B:696:TRP:HB2	1:B:729:PHE:CZ	2.56	0.40
1:B:562:THR:HG21	1:B:669:LEU:HD22	2.03	0.40
1:C:532:MET:O	1:C:717:ILE:HA	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	704/761 (92%)	678 (96%)	23 (3%)	3 (0%)	39	74
1	B	721/761 (95%)	692 (96%)	24 (3%)	5 (1%)	26	63
1	C	704/761 (92%)	680 (97%)	21 (3%)	3 (0%)	39	74
1	D	721/761 (95%)	688 (95%)	27 (4%)	6 (1%)	24	60
All	All	2850/3044 (94%)	2738 (96%)	95 (3%)	17 (1%)	30	67

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	151	ASN
1	B	162	TYR
1	B	163	ALA
1	D	151	ASN
1	D	175	ASP
1	A	724	LYS
1	B	350	ASN
1	C	162	TYR
1	D	156	LYS

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Mol	Chain	Res	Type
1	D	408	LYS
1	D	725	ARG
1	A	574	LYS
1	B	408	LYS
1	C	574	LYS
1	D	176	ASN
1	A	407	PRO
1	C	407	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	573/614 (93%)	548 (96%)	25 (4%)	35	70
1	B	585/614 (95%)	560 (96%)	25 (4%)	35	71
1	C	573/614 (93%)	553 (96%)	20 (4%)	43	78
1	D	585/614 (95%)	557 (95%)	28 (5%)	31	67
All	All	2316/2456 (94%)	2218 (96%)	98 (4%)	36	73

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	THR
1	A	44	ARG
1	A	78	ASP
1	A	120	THR
1	A	131	LEU
1	A	154	ILE
1	A	155	ASP
1	A	161	LYS
1	A	164	TYR
1	A	175	ASP
1	A	193	ARG
1	A	203	THR
1	A	209	GLN

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Mol	Chain	Res	Type
1	A	257	SER
1	A	337	THR
1	A	340	THR
1	A	355	LEU
1	A	377	GLN
1	A	409	THR
1	A	453	PHE
1	A	486	LYS
1	A	574	LYS
1	A	576	ARG
1	A	596	LEU
1	A	713	THR
1	B	44	ARG
1	B	91	THR
1	B	108	LEU
1	B	112	CYS
1	B	135	ASN
1	B	147	GLU
1	B	148	LEU
1	B	162	TYR
1	B	193	ARG
1	B	208	HIS
1	B	209	GLN
1	B	277	ASP
1	B	294	THR
1	B	298	TYR
1	B	337	THR
1	B	358	MET
1	B	453	PHE
1	B	460	GLU
1	B	470	THR
1	B	576	ARG
1	B	596	LEU
1	B	616	GLN
1	B	689	ILE
1	B	703	GLU
1	B	713	THR
1	C	25	SER
1	C	145	LEU
1	C	155	ASP
1	C	159	VAL
1	C	162	TYR

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Mol	Chain	Res	Type
1	C	175	ASP
1	C	193	ARG
1	C	220	HIS
1	C	345	VAL
1	C	401	LEU
1	C	408	LYS
1	C	426	ASN
1	C	453	PHE
1	C	574	LYS
1	C	576	ARG
1	C	596	LEU
1	C	617	SER
1	C	712	THR
1	C	725	ARG
1	C	738	GLN
1	D	44	ARG
1	D	85	ILE
1	D	128	ASP
1	D	131	LEU
1	D	154	ILE
1	D	164	TYR
1	D	193	ARG
1	D	204	THR
1	D	250	GLU
1	D	265	ARG
1	D	266	LEU
1	D	268	ILE
1	D	278	THR
1	D	298	TYR
1	D	308	VAL
1	D	333	LEU
1	D	350	ASN
1	D	362	GLN
1	D	385	ARG
1	D	408	LYS
1	D	442	ARG
1	D	453	PHE
1	D	491	ILE
1	D	576	ARG
1	D	596	LEU
1	D	616	GLN
1	D	671	HIS

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Mol	Chain	Res	Type
1	D	723	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	307	HIS
1	A	392	ASN
1	B	73	ASN
1	B	153	GLN
1	B	209	GLN
1	B	259	ASN
1	B	267	ASN
1	B	667	ASN
1	C	121	ASN
1	C	166	ASN
1	C	392	ASN
1	D	350	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

8 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	PO4	A	801	-	4,4,4	0.47	0	6,6,6	0.27	0
2	PO4	A	802	-	4,4,4	0.51	0	6,6,6	0.27	0
2	PO4	B	801	-	4,4,4	0.48	0	6,6,6	0.27	0
2	PO4	B	802	-	4,4,4	0.49	0	6,6,6	0.27	0
2	PO4	C	801	-	4,4,4	0.48	0	6,6,6	0.27	0
2	PO4	C	802	-	4,4,4	0.49	0	6,6,6	0.27	0
2	PO4	D	801	-	4,4,4	0.50	0	6,6,6	0.28	0
2	PO4	D	802	-	4,4,4	0.47	0	6,6,6	0.27	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
2	PO4	A	801	-	-	0/0/0/0	0/0/0/0
2	PO4	A	802	-	-	0/0/0/0	0/0/0/0
2	PO4	B	801	-	-	0/0/0/0	0/0/0/0
2	PO4	B	802	-	-	0/0/0/0	0/0/0/0
2	PO4	C	801	-	-	0/0/0/0	0/0/0/0
2	PO4	C	802	-	-	0/0/0/0	0/0/0/0
2	PO4	D	801	-	-	0/0/0/0	0/0/0/0
2	PO4	D	802	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	801	PO4	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	712/761 (93%)	-0.21	7 (0%) 84 82	43, 79, 129, 304	0
1	B	727/761 (95%)	-0.05	22 (3%) 54 47	43, 89, 173, 261	0
1	C	712/761 (93%)	-0.16	10 (1%) 78 76	55, 91, 139, 253	0
1	D	727/761 (95%)	-0.05	18 (2%) 61 55	51, 93, 169, 290	0
All	All	2878/3044 (94%)	-0.12	57 (1%) 68 64	43, 88, 157, 304	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	164	TYR	7.6
1	D	164	TYR	7.4
1	C	164	TYR	6.2
1	D	162	TYR	5.8
1	B	154	ILE	5.6
1	A	162	TYR	5.3
1	D	163	ALA	5.0
1	B	153	GLN	4.4
1	B	164	TYR	4.1
1	B	176	ASN	3.6
1	B	141	TRP	3.5
1	C	162	TYR	3.5
1	A	122	LEU	3.5
1	B	205	ALA	3.5
1	B	134	ALA	3.4
1	B	163	ALA	3.2
1	D	453	PHE	3.1
1	B	182	ASP	3.1
1	D	376	PHE	3.1
1	D	176	ASN	2.9
1	A	177	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	298	TYR	2.8
1	A	307	HIS	2.8
1	B	151	ASN	2.8
1	C	358	MET	2.7
1	D	160	GLN	2.6
1	D	525	HIS	2.6
1	D	155	ASP	2.6
1	B	144	LEU	2.5
1	C	629	THR	2.4
1	C	208	HIS	2.4
1	D	444	LEU	2.4
1	B	244	PRO	2.4
1	C	760	ILE	2.4
1	D	265	ARG	2.4
1	C	142	SER	2.4
1	B	206	GLN	2.3
1	B	105	GLU	2.3
1	D	458	ILE	2.3
1	B	512	TYR	2.3
1	D	205	ALA	2.2
1	B	160	GLN	2.2
1	C	353	VAL	2.2
1	D	208	HIS	2.2
1	A	77	ALA	2.2
1	B	156	LYS	2.1
1	D	131	LEU	2.1
1	D	156	LYS	2.1
1	C	457	GLN	2.1
1	A	570	ALA	2.1
1	B	152	GLY	2.1
1	D	711	PHE	2.1
1	B	162	TYR	2.1
1	B	236	TRP	2.0
1	B	177	ASP	2.0
1	D	368	GLN	2.0
1	C	151	ASN	2.0

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

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

### 6.3 Carbohydrates [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	PO4	C	801	5/5	0.96	0.24	2.00	98,99,101,103	0
2	PO4	B	802	5/5	0.96	0.19	0.99	85,85,87,88	0
2	PO4	A	801	5/5	0.91	0.18	0.87	92,97,101,102	0
2	PO4	B	801	5/5	0.95	0.17	0.85	98,100,100,101	0
2	PO4	D	802	5/5	0.97	0.18	0.70	100,100,102,103	0
2	PO4	C	802	5/5	0.96	0.14	-0.25	87,92,93,96	0
2	PO4	A	802	5/5	0.98	0.13	-0.73	70,70,72,77	0
2	PO4	D	801	5/5	0.98	0.11	-1.37	95,96,99,99	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.