



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:45 AM UTC

PDB ID : 4WL0 / pdb_00004wl0
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

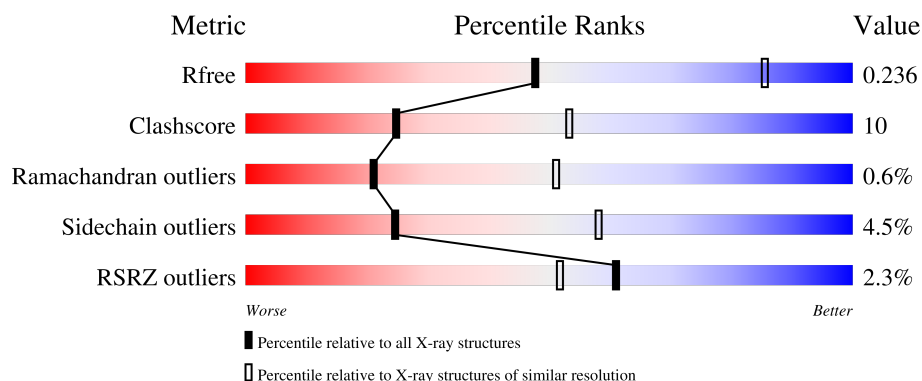
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

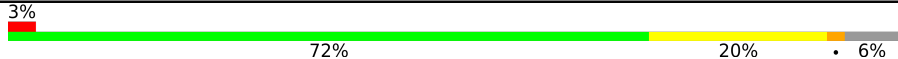
The reported resolution of this entry is 2.89 Å.

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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	761	 3% 72% 20% 6%
1	B	761	 3% 73% 21% 6%
1	C	761	 2% 71% 20% 6%
1	D	761	 % 72% 22% 6%

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 (CCD ID: PO4) (formula: O₄P).

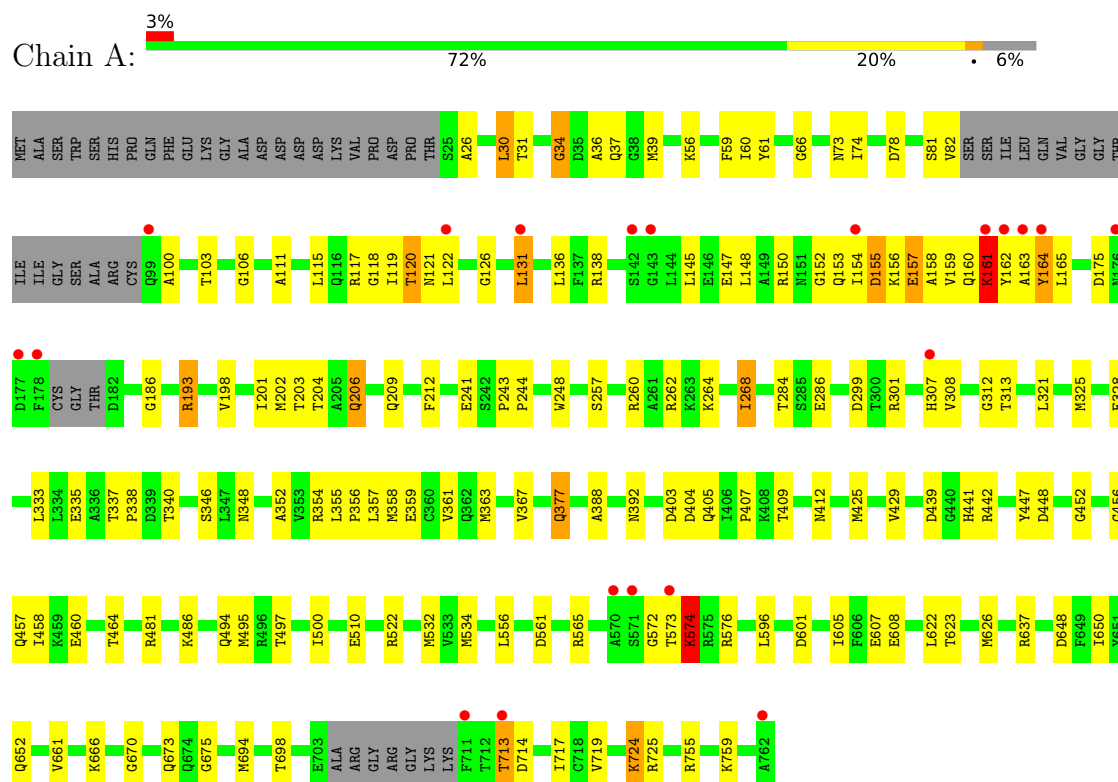


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

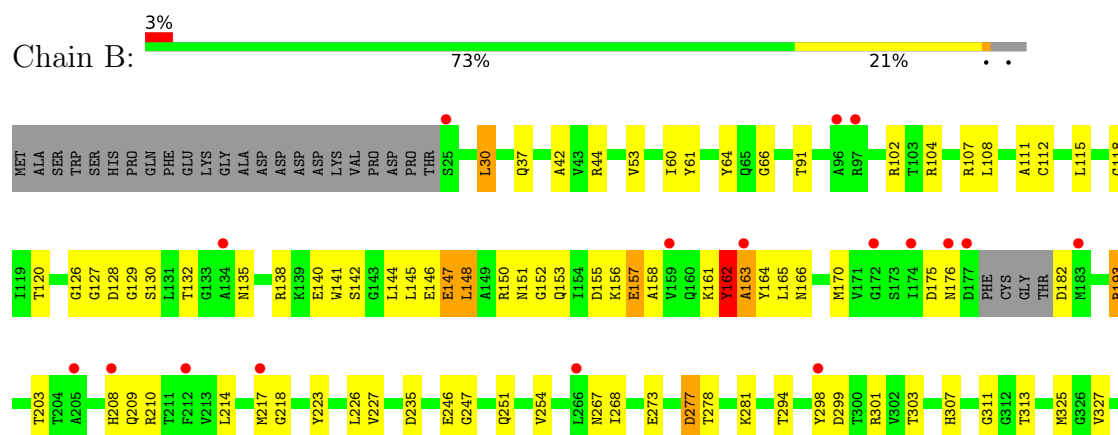
3 Residue-property plots [i](#)

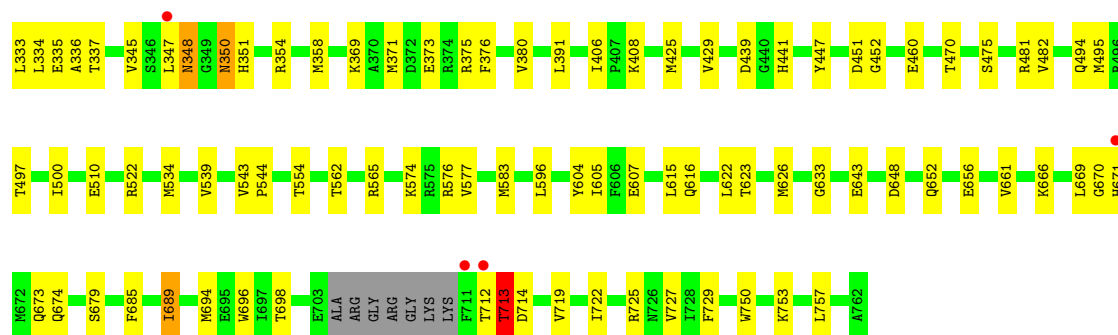
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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

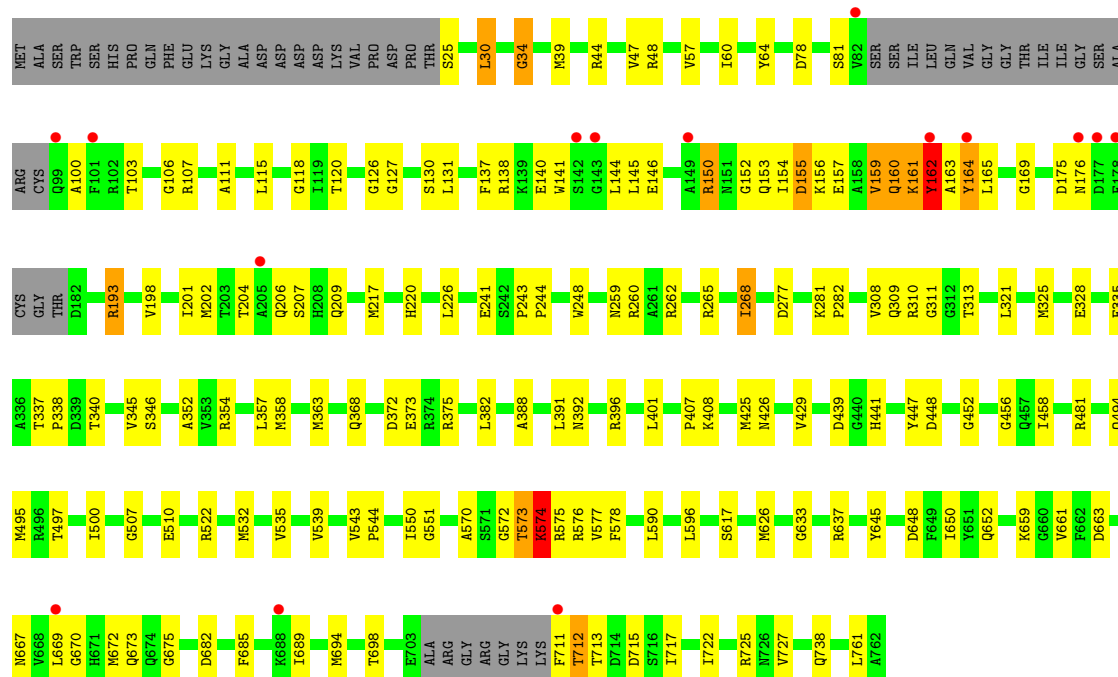


- Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type

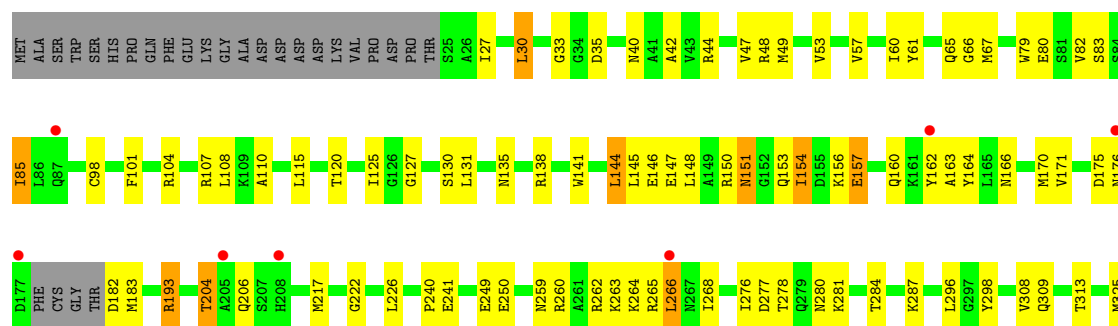


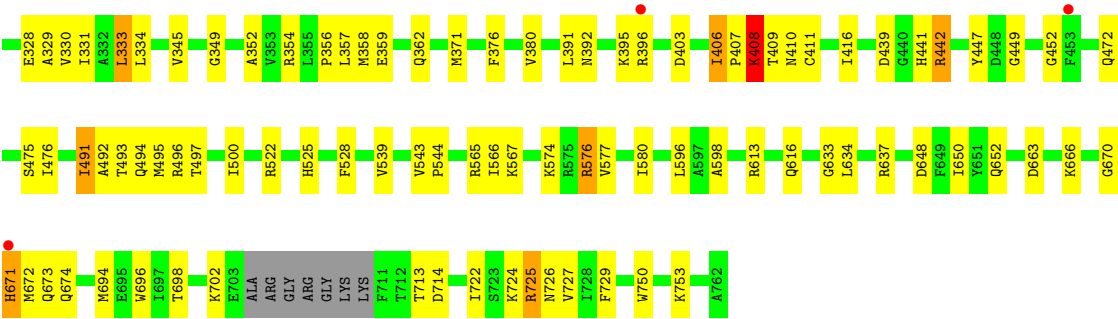


- Molecule 1: ATP-dependent 6-phosphofructokinase, platelet type



- 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, α , β , γ	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) 99.6 (46.97-2.89)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	3991 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	67.7	Xtriage
Anisotropy	0.829	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 60.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22052	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.39	0/5539	0.87	6/7480 (0.1%)
1	B	0.41	1/5642 (0.0%)	0.88	9/7620 (0.1%)
1	C	0.40	1/5539 (0.0%)	0.89	11/7480 (0.1%)
1	D	0.38	0/5642	0.85	6/7620 (0.1%)
All	All	0.39	2/22362 (0.0%)	0.87	32/30200 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	161	LYS	CA-C	8.56	1.61	1.52
1	B	713	THR	CA-CB	5.76	1.63	1.53

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	160	GLN	N-CA-C	-12.29	97.56	111.82
1	C	161	LYS	N-CA-C	9.29	124.61	112.72
1	C	164	TYR	CA-C-N	-8.48	111.06	122.85
1	C	164	TYR	C-N-CA	-8.48	111.06	122.85
1	D	206	GLN	N-CA-C	-8.28	102.96	113.23
1	A	161	LYS	N-CA-C	7.57	123.44	113.30
1	D	157	GLU	N-CA-C	-7.46	103.13	112.90
1	B	348	ASN	N-CA-C	-6.99	104.68	112.57
1	A	160	GLN	N-CA-C	-6.69	104.06	111.82
1	B	157	GLU	N-CA-C	-6.66	104.17	112.90
1	B	406	ILE	CA-C-N	6.64	127.18	119.47
1	B	406	ILE	C-N-CA	6.64	127.18	119.47
1	D	160	GLN	N-CA-C	6.51	118.45	111.36
1	B	712	THR	CA-C-N	6.28	133.53	121.54
1	B	712	THR	C-N-CA	6.28	133.53	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	152	GLY	N-CA-C	6.12	121.26	113.24
1	C	34	GLY	N-CA-C	5.97	119.66	111.54
1	D	406	ILE	CA-C-N	5.83	127.12	119.84
1	D	406	ILE	C-N-CA	5.83	127.12	119.84
1	A	157	GLU	N-CA-C	-5.78	105.33	112.90
1	A	34	GLY	N-CA-C	5.74	119.35	111.54
1	B	126	GLY	N-CA-C	5.73	118.59	110.74
1	C	507	GLY	N-CA-C	5.54	118.61	110.80
1	C	659	LYS	N-CA-C	5.51	117.73	111.11
1	C	150	ARG	N-CA-C	-5.41	102.75	110.59
1	C	126	GLY	N-CA-C	5.30	118.00	110.74
1	C	176	ASN	N-CA-C	5.22	116.52	109.11
1	A	126	GLY	N-CA-C	5.21	117.87	110.74
1	B	713	THR	N-CA-CB	5.20	119.28	110.49
1	D	33	GLY	N-CA-C	5.12	117.50	111.35
1	B	278	THR	N-CA-C	-5.04	106.96	113.01
1	A	157	GLU	N-CA-CB	5.02	117.86	110.33

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	102	0
1	B	5554	0	5579	109	0
1	C	5452	0	5465	125	0
1	D	5554	0	5579	115	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	431	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 10.

All (431) 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: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:669:LEU:HA	1:D:672:MET:HE1	1.63	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:B:348:ASN:HB3	1:B:725:ARG:NH2	2.05	0.72
1:D:138:ARG:HH12	1:D:166:ASN:HA	1.55	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
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:34:GLY:HA3	1:C:39:MET:HE1	1.73	0.69
1:C:388:ALA:O	1:C:392:ASN:ND2	2.26	0.69
1:C:217:MET:HE1	1:C:310:ARG:HG3	1.73	0.68
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:A:494:GLN:HA	1:A:497:THR:HG22	1.78	0.66
1:D:522:ARG:NH1	1:D:713:THR:O	2.29	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:A:34:GLY:HA3	1:A:39:MET:HE1	1.79	0.64
1:C:78:ASP:OD1	1:C:81:SER:OG	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ARG:HA	1:A:165:LEU:HD23	1.80	0.64
1:A:198:VAL:HG12	1:A:202:MET:HE2	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:B:162:TYR:C	1:B:164:TYR:H	2.07	0.62
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:363:MET:HE1	1:C:382:LEU:HD22	1.83	0.61
1:B:441:HIS:NE2	1:B:698:THR:HG22	2.15	0.61
1:C:144:LEU:HD21	1:C:164:TYR:HE2	1.65	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:A:74:ILE:HD11	1:A:117:ARG:NE	2.17	0.60
1:C:663:ASP:OD1	1:C:663:ASP:N	2.34	0.60
1:B:210:ARG:NH1	1:B:299:ASP:OD2	2.35	0.60
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:OE1	1:C:157:GLU:N	2.35	0.59
1:B:144:LEU:HD21	1:B:158:ALA:HA	1.83	0.59
1:B:102:ARG:C	1:B:107:ARG:HH21	2.10	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:A:441:HIS:NE2	1:A:698:THR:HG22	2.19	0.58
1:B:166:ASN:ND2	1:B:333:LEU:O	2.36	0.58
1:B:750:TRP:O	1:B:753:LYS:HG2	2.03	0.58
1:C:48:ARG:NH1	1:C:761:LEU:O	2.36	0.58
1:B:155:ASP:C	1:B:157:GLU:H	2.10	0.58
1:B:64:TYR:OH	1:B:130:SER:O	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:325:MET:HE1	1:C:346:SER:HA	1.86	0.56
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:C:669:LEU:HD23	1:D:672:MET:HE1	1.88	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:A:164:TYR:C	1:A:164:TYR:HD1	2.14	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:A:573:THR:O	1:A:574:LYS:HG2	2.06	0.55
1:C:439:ASP:OD2	1:C:698:THR:HG21	2.07	0.55
1:C:522:ARG:NH1	1:C:713:THR:O	2.40	0.55
1:B:148:LEU:HD11	1:B:158:ALA:HB2	1.89	0.55
1:D:410:ASN:HA	1:D:442:ARG:NH1	2.22	0.55
1:D:493:THR:O	1:D:496:ARG:HG2	2.07	0.55
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:321:LEU:HD11	1:C:325:MET:HE2	1.89	0.54
1:D:441:HIS:NE2	1:D: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:C:441:HIS:NE2	1:C:698:THR:HG22	2.22	0.54
1:A:675:GLY:HA2	1:B:565:ARG:NH1	2.22	0.54
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:B:251:GLN:O	1:B:254:VAL:HG12	2.07	0.54
1:C:131:LEU:HD22	1:C:169:GLY:HA3	1.89	0.54
1:D:567:LYS:NZ	1:D:598:ALA:O	2.28	0.54
1:A:159:VAL:HA	1:A:162:TYR:CE2	2.43	0.54
1:C:141:TRP:CZ2	1:C:164:TYR:CZ	2.95	0.54
1:B:135:ASN:O	1:B:138:ARG:HB3	2.08	0.54
1:A:605:ILE:HD12	1:A:607:GLU:HB2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:198:VAL:HG12	1:C:202:MET:HE2	1.90	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:204:THR:C	1:C:206:GLN:H	2.17	0.53
1:A:164:TYR:C	1:A:164:TYR:CD1	2.87	0.53
1:A:325:MET:HE1	1:A:346:SER:HA	1.90	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:A:284:THR:HB	1:A:286:GLU:OE1	2.09	0.52
1:C:685:PHE:O	1:C:689:ILE:HG12	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:A:321:LEU:HD11	1:A:325:MET:HE2	1.92	0.52
1:D:577:VAL:HG22	1:D:633:GLY:HA3	1.91	0.52
1:A:495:MET:HG2	1:A:500:ILE:HD12	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:34:GLY:HA3	1:A:39:MET:CE	2.38	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:C:578:PHE:HE2	1:D:671:HIS:CE1	2.27	0.51
1:D:153:GLN:N	1:D:153:GLN:OE1	2.44	0.51
1:C:447:TYR:O	1:C:452:GLY:HA3	2.10	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:145:LEU:HD23	1:A:148:LEU:HD21	1.93	0.50
1:B:115:LEU:HD11	1:B:144:LEU:HD12	1.94	0.50
1:B:277:ASP:N	1:B:281:LYS:O	2.44	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:A:30:LEU:HB3	1:A:60:ILE:HB	1.94	0.50
1:A:623:THR:HG23	1:A:661:VAL:HG21	1.93	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: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:A:358:MET:HA	1:A:361:VAL:HG22	1.94	0.50
1:C:713:THR:OG1	1:C:715:ASP:OD1	2.26	0.50
1:B:214:LEU:HD22	1:B:303:THR:HB	1.93	0.50
1:B:144:LEU:C	1:B:144:LEU:HD23	2.37	0.49
1:D:42:ALA:HB1	1:D:170:MET:HE1	1.94	0.49
1:D:145:LEU:O	1:D:148:LEU:HG	2.12	0.49
1:C:575:ARG:HH12	1:C:661:VAL:HG13	1.77	0.49
1:C:670:GLY:O	1:C:673:GLN:HG3	2.12	0.49
1:A:670:GLY:O	1:A:673:GLN:HG3	2.11	0.49
1:B:162:TYR:O	1:B:164:TYR:N	2.46	0.49
1:B:347:LEU:HG	1:B:350:ASN:H	1.78	0.49
1:C:202:MET:HG2	1:C:268:ILE:HD11	1.93	0.49
1:C:575:ARG:HD3	1:C:661:VAL:O	2.13	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: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: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
1:A:206:GLN:N	1:A:206:GLN:OE1	2.46	0.48
1:A:404:ASP:OD1	1:A:405:GLN:HG3	2.13	0.48
1:D:403:ASP:O	1:D:408:LYS:NZ	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:439:ASP:OD2	1:B:698:THR:HG21	2.14	0.48
1:C:131:LEU:HG	1:C:357:LEU:HD22	1.95	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:622:LEU:O	1:A:626:MET:HG2	2.14	0.48
1:A:356:PRO:HG2	1:A:359:GLU:CD	2.39	0.47
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:A:37:GLN:HE22	1:B:203:THR:HG22	1.79	0.47
1:A:147:GLU:HB2	1:A:153:GLN:HE21	1.78	0.47
1:C:161:LYS:O	1:C:164:TYR:HD2	1.98	0.47
1:C:711:PHE:O	1:C:712:THR:HG23	2.15	0.47
1:D:260:ARG:HD3	1:D:298:TYR:CZ	2.49	0.47
1:B:577:VAL:HG22	1:B:633:GLY:HA3	1.97	0.47
1:C:667:ASN:HB3	1:D:672:MET:HE2	1.96	0.47
1:A:363:MET:O	1:A:367:VAL:HG23	2.15	0.47
1:B:135:ASN:C	1:B:135:ASN:HD22	2.21	0.47
1:B:685:PHE:CE2	1:B:689:ILE:HG13	2.49	0.47
1:C:241:GLU:O	1:C:243:PRO:HD3	2.14	0.47
1:A:608:GLU:CD	1:A:755:ARG:HH21	2.23	0.47
1:C:675:GLY:HA2	1:D:565:ARG:HH11	1.78	0.47
1:D:447:TYR:O	1:D:452:GLY:HA3	2.14	0.47
1:D:525:HIS:HB2	1:D:528:PHE:CE2	2.50	0.47
1:A:439:ASP:OD2	1:A:698:THR:HG21	2.15	0.47
1:B:145:LEU:HB3	1:B:162:TYR:OH	2.15	0.47
1:C:141:TRP:O	1:C:144:LEU:HD13	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:HA	1:B:193:ARG:HD3	1.64	0.46
1:D:222:GLY:HA3	1:D:240:PRO:HD2	1.97	0.46
1:D:406:ILE:HB	1:D:408:LYS:NZ	2.29	0.46
1:B:129:GLY:HA2	1:B:132:THR:HG23	1.97	0.46
1:B:166:ASN:ND2	1:B:336:ALA:HB3	2.30	0.46
1:D:328:GLU:HG2	1:D:352:ALA:HB1	1.96	0.46
1:A:601:ASP:O	1:A:759:LYS:NZ	2.33	0.46
1:B:156:LYS:HE2	1:B:156:LYS:HB2	1.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:GLN:OE1	1:B:298:TYR:OH	2.32	0.46
1:C:675:GLY:HA2	1:D:565:ARG:NH1	2.31	0.46
1:A:456:GLY:HA2	1:A:458:ILE:HD12	1.97	0.46
1:D:580:ILE:HD12	1:D:634:LEU:HD11	1.98	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:C:572:GLY:HA3	1:D:475:SER:O	2.16	0.45
1:D:80:GLU:O	1:D:83:SER:OG	2.31	0.45
1:A:111:ALA:O	1:A:115:LEU:HG	2.16	0.45
1:B:108:LEU:HD13	1:B:150:ARG:HH21	1.82	0.45
1:B:226:LEU:HD11	1:B:391:LEU:HA	1.99	0.45
1:C:103:THR:HG23	1:C:106:GLY:H	1.81	0.45
1:D:439:ASP:OD2	1:D:698:THR:HG21	2.16	0.45
1:A:481:ARG:NH1	1:A:510:GLU:OE2	2.49	0.45
1:C:78:ASP:N	1:C:81:SER:OG	2.39	0.45
1:D:241:GLU:HG3	1:D:371:MET:HE1	1.97	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:D:296:LEU:HB3	1:D:298:TYR:CD2	2.50	0.45
1:B:451:ASP:HB2	1:B:482:VAL:HG11	1.98	0.45
1:B:622:LEU:O	1:B:626:MET:HG2	2.16	0.45
1:D:193:ARG:HD3	1:D:193:ARG:HA	1.68	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:D:260:ARG:C	1:D:263:LYS:H	2.25	0.45
1:A:648:ASP:OD1	1:A:666:LYS:NZ	2.26	0.45
1:C:47:VAL:HA	1:C:57:VAL:HG11	1.98	0.45
1:D:67:MET:HG2	1:D:110:ALA:HB1	1.99	0.45
1:A:209:GLN:HG2	1:A:260:ARG:NH2	2.31	0.44
1:B:583:MET:HG3	1:B:673:GLN:NE2	2.33	0.44
1:C:281:LYS:HG3	1:C:282:PRO:HD2	1.99	0.44
1:C:577:VAL:HG22	1:C:633:GLY:HA3	1.99	0.44
1:D:138:ARG:NH1	1:D:166:ASN:HA	2.28	0.44
1:A:425:MET:O	1:A:429:VAL:HG23	2.17	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:B:605:ILE:HD12	1:B:607:GLU:HB2	1.99	0.44
1:C:64:TYR:OH	1:C:130:SER:O	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:THR:HB	1:A:164:TYR:CE1	2.52	0.44
1:A:156:LYS:HD2	1:A:156:LYS:N	2.31	0.44
1:C:163:ALA:HB1	1:C:338:PRO:HB3	2.00	0.44
1:A:26:ALA:HB3	1:A:119:ILE:HA	1.98	0.44
1:A:122:LEU:HD23	1:A:122:LEU:HA	1.81	0.44
1:B:246:GLU:HA	1:B:247:GLY:HA2	1.66	0.44
1:C:144:LEU:HD11	1:C:164:TYR:HH	1.83	0.44
1:C:217:MET:HE3	1:C:309:GLN:HB2	2.00	0.44
1:D:491:ILE:HG13	1:D:492:ALA:N	2.32	0.44
1:D:713:THR:OG1	1:D:714:ASP:N	2.50	0.44
1:D:108:LEU:HD21	1:D:146:GLU:CD	2.43	0.44
1:C:495:MET:HA	1:C:500:ILE:HD12	1.99	0.44
1:C:590:LEU:HD12	1:C:590:LEU:H	1.82	0.44
1:D:141:TRP:HD1	1:D:163:ALA:H	1.65	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:A:100:ALA:O	1:A:103:THR:HG22	2.17	0.43
1:C:141:TRP:CZ2	1:C:164:TYR:CE1	3.05	0.43
1:C:141:TRP:CE3	1:C:165:LEU:HD22	2.53	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:A:56:LYS:HD2	1:A:56:LYS:HA	1.84	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:D:264:LYS:NZ	2:D:801:PO4:O2	2.31	0.43
1:B:162:TYR:C	1:B:164:TYR:N	2.75	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:B:425:MET:O	1:B:429:VAL:HG23	2.18	0.43
1:C:358:MET:HE3	1:C:358:MET:HB2	1.76	0.43
1:D:566:ILE:HD13	1:D:580:ILE:CD1	2.48	0.43
1:D:750:TRP:O	1:D:753:LYS:HG2	2.17	0.43
1:A:725:ARG:O	1:A:725:ARG:HG2	2.18	0.43
1:A:131:LEU:H	1:A:131:LEU:HG	1.45	0.43
1:B:583:MET:HE2	1:B:673:GLN:HG3	2.00	0.43
1:C:160:GLN:C	1:C:161:LYS:HG2	2.44	0.43
1:D:47:VAL:HA	1:D:57:VAL:HG11	2.01	0.43
1:D:277:ASP:N	1:D:281:LYS:O	2.47	0.43
1:A:138:ARG:HG3	1:A:165:LEU:O	2.17	0.43
1:A:201:ILE:O	1:A:204:THR:HG22	2.19	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:D:329:ALA:HA	1:D:345:VAL:HG11	2.00	0.43
1:B:210:ARG:NH1	1:B:299:ASP:CG	2.77	0.43
1:B:583:MET:SD	1:B:671:HIS:HA	2.59	0.43
1:C:335:GLU:CD	1:C:354:ARG:HH22	2.26	0.43
1:D:543:VAL:HA	1:D:544:PRO:HD3	1.91	0.43
1:C:159:VAL:C	1:C:161:LYS:N	2.69	0.42
1:C:161:LYS:O	1:C:162:TYR:C	2.61	0.42
1:C:551:GLY:H	1:C:682:ASP:CG	2.27	0.42
1:C:672:MET:HB2	1:C:672:MET:HE3	1.76	0.42
1:A:121:ASN:HB3	1:A:333:LEU:HD22	2.01	0.42
1:B:543:VAL:HA	1:B:544:PRO:HD3	1.92	0.42
1:B:554:THR:HG1	1:B:679:SER:H	1.65	0.42
1:D:48:ARG:HD3	1:D:79:TRP:CZ2	2.54	0.42
1:D:150:ARG:NH1	1:D:151:ASN:OD1	2.52	0.42
1:A:150:ARG:NH1	1:A:152:GLY:HA3	2.33	0.42
1:B:481:ARG:HH11	1:B:510:GLU:CD	2.28	0.42
1:D:722:ILE:HG12	1:D:727:VAL:HG12	2.00	0.42
1:B:510:GLU:CD	1:B:510:GLU:H	2.26	0.42
1:D:44:ARG:HA	1:D:82:VAL:HG11	2.00	0.42
1:D:49:MET:HB3	1:D:330:VAL:HG21	2.02	0.42
1:C:34:GLY:HA3	1:C:39:MET:CE	2.46	0.42
1:C:226:LEU:HD11	1:C:391:LEU:HA	2.01	0.42
1:D:325:MET:HE2	1:D:325:MET:HA	2.02	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:A:118:GLY:O	1:A:120:THR:HG22	2.20	0.42
1:B:37:GLN:NE2	1:B:311:GLY:O	2.51	0.42
1:B:164:TYR:N	1:B:164:TYR:CD2	2.87	0.42
1:C:138:ARG:HA	1:C:165:LEU:HD23	2.02	0.42
1:D:406:ILE:HA	1:D:407:PRO:HD2	1.88	0.42
1:A:153:GLN:HB2	1:A:157:GLU:OE1	2.20	0.42
1:A:163:ALA:O	1:A:338:PRO:HB3	2.20	0.42
1:A:312:GLY:O	1:B:203:THR:HG21	2.19	0.42
1:B:128:ASP:OD1	1:B:128:ASP:N	2.51	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: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:193:ARG:HA	1:C:193:ARG:HD3	1.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:MET:HA	1:A:500:ILE:HD12	2.01	0.41
1:A:556:LEU:HD23	1:A:556:LEU:HA	1.91	0.41
1:B:235:ASP:OD2	1:B:267:ASN:HA	2.21	0.41
1:C:120:THR:HB	1:C:164:TYR:HD1	1.84	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:127:GLY:O	1:C:130:SER:OG	2.30	0.41
1:C:543:VAL:HA	1:C:544:PRO:HD3	1.94	0.41
1:D:141:TRP:HE1	1:D:162:TYR:HA	1.86	0.41
1:D:144:LEU:HA	1:D:147:GLU:OE1	2.19	0.41
1:C:162:TYR:O	1:C:163:ALA:HB3	2.20	0.41
1:D:416:ILE:HD11	1:D:449:GLY:C	2.45	0.41
1:A:532:MET:O	1:A:717:ILE:HA	2.21	0.41
1:B:335:GLU:CD	1:B:354:ARG:HH22	2.29	0.41
1:B:495:MET:HA	1:B:500:ILE:HD12	2.03	0.41
1:D:170:MET:HE3	1:D:325:MET:CB	2.51	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:C:209:GLN:HG2	1:C:265:ARG:HA	2.03	0.41
1:D:331:ILE:HG22	1:D:354:ARG:NH2	2.36	0.41
1:D:396:ARG:HG3	1:D:396:ARG:HH11	1.85	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:A:412:ASN:OD1	1:A:442:ARG:HB3	2.21	0.41
1:B:175:ASP:OD1	1:B:176:ASN:N	2.53	0.41
1:B:447:TYR:O	1:B:452:GLY:HA3	2.21	0.41
1:B:604:TYR:CZ	1:B:615:LEU:HD23	2.56	0.41
1:C:44:ARG:HH21	1:C:48:ARG:HH12	1.69	0.41
1:C:120:THR:HG22	1:C:164:TYR:CD1	2.55	0.41
1:D:376:PHE:O	1:D:380:VAL:HG23	2.21	0.41
1:A:61:TYR:N	1:A:73:ASN:O	2.48	0.41
1:B:155:ASP:C	1:B:157:GLU:N	2.78	0.41
1:B:182:ASP:OD1	1:B:348:ASN:HA	2.21	0.41
1:B:223:TYR:CZ	1:B:227:VAL:HG21	2.55	0.41
1:B:375:ARG:HH11	1:B:375:ARG:HD2	1.73	0.41
1:C:165:LEU:HD12	1:C:165:LEU:HA	1.76	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:C:722:ILE:HG12	1:C:727:VAL:HG12	2.03	0.41
1:A:335:GLU:CD	1:A:354:ARG:HH22	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:GLN:H	1:A:377:GLN:HG2	1.61	0.41
1:A:675:GLY:HA2	1:B:565:ARG:HH11	1.85	0.41
1:B:325:MET:HE2	1:B:325:MET:HA	2.02	0.41
1:C:669:LEU:HD23	1:D:672:MET:CE	2.50	0.41
1:B:165:LEU:HD12	1:B:165:LEU:HA	1.94	0.40
1:D:411:CYS:O	1:D:442:ARG:HG2	2.21	0.40
1:D:637:ARG:HD2	1:D:650:ILE:HD12	2.03	0.40
1:A:136:LEU:HD23	1:A:136:LEU:HA	1.86	0.40
1:B:42:ALA:HB1	1:B:170:MET:HE1	2.03	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:61:TYR:O	1:D:66:GLY:HA3	2.21	0.40
1:D:613:ARG:H	1:D:613:ARG:HG2	1.67	0.40
1:D:702:LYS:HD2	1:D:702:LYS:HA	1.82	0.40
1:B:127:GLY:O	1:B:130:SER:OG	2.39	0.40
1:B:155:ASP:CG	1:B:156:LYS:H	2.30	0.40
1:B:562:THR:HG21	1:B:669:LEU:HD22	2.03	0.40
1:B:696:TRP:HB2	1:B:729:PHE:CZ	2.56	0.40
1:C:204:THR:C	1:C:206:GLN:N	2.80	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%)	30 59
1	B	721/761 (95%)	692 (96%)	24 (3%)	5 (1%)	18 48
1	C	704/761 (92%)	680 (97%)	21 (3%)	3 (0%)	30 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	721/761 (95%)	688 (95%)	27 (4%)	6 (1%)	16	44
All	All	2850/3044 (94%)	2738 (96%)	95 (3%)	17 (1%)	21	51

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
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%)	546 (95%)	27 (5%)	23	56
1	B	585/614 (95%)	558 (95%)	27 (5%)	24	57
1	C	573/614 (93%)	550 (96%)	23 (4%)	28	62
1	D	585/614 (95%)	558 (95%)	27 (5%)	24	57
All	All	2316/2456 (94%)	2212 (96%)	104 (4%)	24	58

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	A	31	THR
1	A	78	ASP
1	A	81	SER
1	A	82	VAL
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	206	GLN
1	A	257	SER
1	A	268	ILE
1	A	337	THR
1	A	340	THR
1	A	355	LEU
1	A	377	GLN
1	A	409	THR
1	A	486	LYS
1	A	574	LYS
1	A	576	ARG
1	A	596	LEU
1	A	713	THR
1	B	30	LEU
1	B	44	ARG
1	B	91	THR
1	B	112	CYS
1	B	120	THR
1	B	147	GLU
1	B	148	LEU
1	B	162	TYR
1	B	193	ARG
1	B	208	HIS
1	B	217	MET
1	B	268	ILE
1	B	277	ASP
1	B	294	THR
1	B	337	THR

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Mol	Chain	Res	Type
1	B	345	VAL
1	B	358	MET
1	B	371	MET
1	B	460	GLU
1	B	470	THR
1	B	576	ARG
1	B	596	LEU
1	B	616	GLN
1	B	643	GLU
1	B	666	LYS
1	B	689	ILE
1	B	713	THR
1	C	25	SER
1	C	30	LEU
1	C	145	LEU
1	C	155	ASP
1	C	159	VAL
1	C	162	TYR
1	C	175	ASP
1	C	193	ARG
1	C	220	HIS
1	C	268	ILE
1	C	308	VAL
1	C	345	VAL
1	C	401	LEU
1	C	408	LYS
1	C	426	ASN
1	C	573	THR
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	30	LEU
1	D	85	ILE
1	D	125	ILE
1	D	131	LEU
1	D	144	LEU
1	D	154	ILE
1	D	171	VAL

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Mol	Chain	Res	Type
1	D	193	ARG
1	D	204	THR
1	D	249	GLU
1	D	250	GLU
1	D	265	ARG
1	D	266	LEU
1	D	268	ILE
1	D	278	THR
1	D	308	VAL
1	D	333	LEU
1	D	362	GLN
1	D	408	LYS
1	D	442	ARG
1	D	491	ILE
1	D	576	ARG
1	D	596	LEU
1	D	616	GLN
1	D	666	LYS
1	D	671	HIS
1	D	726	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	135	ASN
1	A	151	ASN
1	A	220	HIS
1	A	280	ASN
1	A	307	HIS
1	A	392	ASN
1	A	494	GLN
1	A	684	ASN
1	A	726	ASN
1	B	153	GLN
1	B	209	GLN
1	B	259	ASN
1	B	267	ASN
1	B	368	GLN
1	B	457	GLN
1	B	494	GLN
1	B	568	GLN

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Mol	Chain	Res	Type
1	B	638	ASN
1	B	684	ASN
1	C	121	ASN
1	C	166	ASN
1	C	307	HIS
1	C	351	HIS
1	C	392	ASN
1	C	494	GLN
1	C	498	HIS
1	C	638	ASN
1	C	652	GLN
1	C	684	ASN
1	D	135	ASN
1	D	307	HIS
1	D	350	ASN
1	D	457	GLN
1	D	568	GLN
1	D	618	ASN
1	D	638	ASN
1	D	684	ASN
1	D	730	GLN
1	D	749	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	C	802	-	4,4,4	0.97	0	6,6,6	0.50	0
2	PO4	C	801	-	4,4,4	0.97	0	6,6,6	0.46	0
2	PO4	D	802	-	4,4,4	0.96	0	6,6,6	0.47	0
2	PO4	D	801	-	4,4,4	0.98	0	6,6,6	0.51	0
2	PO4	A	802	-	4,4,4	0.98	0	6,6,6	0.51	0
2	PO4	B	802	-	4,4,4	0.98	0	6,6,6	0.46	0
2	PO4	A	801	-	4,4,4	0.95	0	6,6,6	0.50	0
2	PO4	B	801	-	4,4,4	0.96	0	6,6,6	0.47	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	712/761 (93%)	-0.04	20 (2%) 55 46	43, 79, 129, 304	0
1	B	727/761 (95%)	0.07	21 (2%) 53 45	43, 89, 173, 261	0
1	C	712/761 (93%)	0.09	15 (2%) 63 54	55, 91, 139, 253	0
1	D	727/761 (95%)	0.04	10 (1%) 73 65	51, 93, 169, 290	0
All	All	2878/3044 (94%)	0.04	66 (2%) 61 52	43, 88, 157, 304	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	176	ASN	5.8
1	B	177	ASP	5.7
1	C	164	TYR	5.2
1	A	178	PHE	5.0
1	D	177	ASP	4.9
1	B	176	ASN	4.4
1	A	177	ASP	4.4
1	C	178	PHE	4.3
1	A	164	TYR	4.2
1	B	266	LEU	4.1
1	A	570	ALA	3.9
1	C	142	SER	3.8
1	D	266	LEU	3.8
1	B	205	ALA	3.7
1	B	183	MET	3.6
1	C	143	GLY	3.6
1	A	176	ASN	3.5
1	C	176	ASN	3.5
1	A	143	GLY	3.4
1	A	162	TYR	3.3
1	B	174	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	99	GLN	3.2
1	C	162	TYR	3.1
1	C	177	ASP	3.1
1	C	688	LYS	3.1
1	A	573	THR	3.0
1	A	131	LEU	3.0
1	B	298	TYR	3.0
1	D	205	ALA	3.0
1	A	711	PHE	2.9
1	A	142	SER	2.8
1	B	25	SER	2.8
1	B	671	HIS	2.8
1	B	134	ALA	2.7
1	B	208	HIS	2.7
1	A	99	GLN	2.7
1	B	347	LEU	2.6
1	B	163	ALA	2.6
1	C	669	LEU	2.6
1	C	149	ALA	2.6
1	A	713	THR	2.5
1	D	453	PHE	2.5
1	B	712	THR	2.5
1	C	711	PHE	2.5
1	A	161	LYS	2.5
1	D	208	HIS	2.5
1	C	101	PHE	2.4
1	B	97	ARG	2.4
1	D	396	ARG	2.3
1	B	96	ALA	2.3
1	D	162	TYR	2.3
1	B	217	MET	2.2
1	A	571	SER	2.2
1	D	87	GLN	2.2
1	A	307	HIS	2.2
1	A	762	ALA	2.2
1	C	82	VAL	2.1
1	B	711	PHE	2.1
1	A	154	ILE	2.1
1	B	172	GLY	2.1
1	C	205	ALA	2.1
1	D	671	HIS	2.1
1	B	159	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	212	PHE	2.1
1	A	122	LEU	2.1
1	A	163	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PO4	B	801	5/5	0.88	0.08	98,100,100,101	0
2	PO4	D	801	5/5	0.89	0.07	95,96,99,99	0
2	PO4	D	802	5/5	0.90	0.09	100,100,102,103	0
2	PO4	A	801	5/5	0.92	0.09	92,97,101,102	0
2	PO4	B	802	5/5	0.93	0.11	85,85,87,88	0
2	PO4	C	802	5/5	0.93	0.07	87,92,93,96	0
2	PO4	C	801	5/5	0.95	0.07	98,99,101,103	0
2	PO4	A	802	5/5	0.97	0.06	70,70,72,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.