



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 05:54 AM GMT

PDB ID : 2I22  
Title : Crystal structure of Escherichia coli phosphoheptose isomerase in complex with reaction substrate sedoheptulose 7-phosphate  
Authors : Blakely, K.; Zhang, K.; DeLeon, G.; Wright, G.; Junop, M.  
Deposited on : 2006-08-15  
Resolution : 2.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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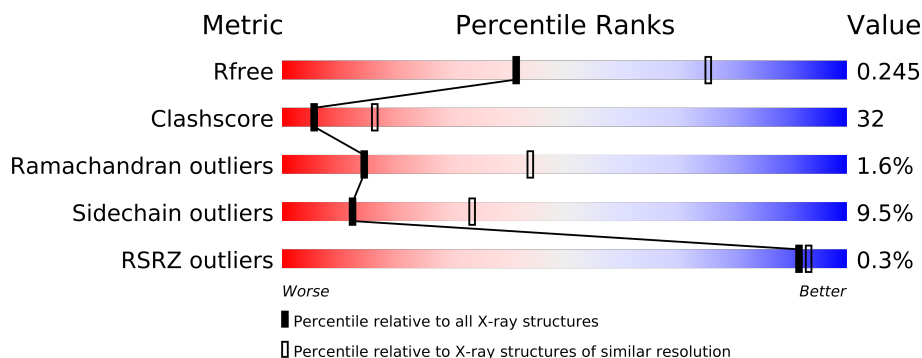
The following versions of software and data (see [references](#)) were used in the production of this report:

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

# 1 Overall quality at a glance

The reported resolution of this entry is 2.80 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	212	
1	B	212	
1	C	212	
1	D	212	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	I22	B	900	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5665 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Phosphoheptose isomerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	0	0	0
			1365	853	245	260	7			
1	B	178	Total	C	N	O	S	0	0	0
			1357	849	244	257	7			
1	C	178	Total	C	N	O	S	0	0	0
			1357	849	244	257	7			
1	D	178	Total	C	N	O	S	0	0	0
			1357	849	244	257	7			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P63224
A	-18	GLY	-	EXPRESSION TAG	UNP P63224
A	-17	SER	-	EXPRESSION TAG	UNP P63224
A	-16	SER	-	EXPRESSION TAG	UNP P63224
A	-15	HIS	-	EXPRESSION TAG	UNP P63224
A	-14	HIS	-	EXPRESSION TAG	UNP P63224
A	-13	HIS	-	EXPRESSION TAG	UNP P63224
A	-12	HIS	-	EXPRESSION TAG	UNP P63224
A	-11	HIS	-	EXPRESSION TAG	UNP P63224
A	-10	HIS	-	EXPRESSION TAG	UNP P63224
A	-9	SER	-	EXPRESSION TAG	UNP P63224
A	-8	SER	-	EXPRESSION TAG	UNP P63224
A	-7	GLY	-	EXPRESSION TAG	UNP P63224
A	-6	LEU	-	EXPRESSION TAG	UNP P63224
A	-5	VAL	-	EXPRESSION TAG	UNP P63224
A	-4	PRO	-	EXPRESSION TAG	UNP P63224
A	-3	ARG	-	EXPRESSION TAG	UNP P63224
A	-2	GLY	-	EXPRESSION TAG	UNP P63224
A	-1	SER	-	EXPRESSION TAG	UNP P63224
A	0	HIS	-	EXPRESSION TAG	UNP P63224
B	-19	MET	-	EXPRESSION TAG	UNP P63224

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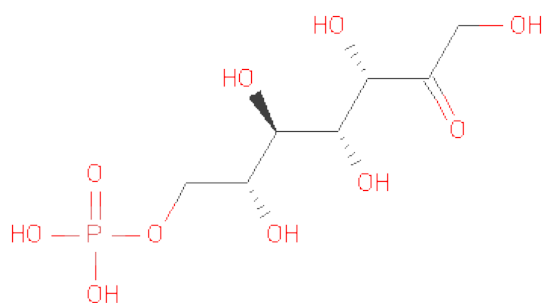
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	EXPRESSION TAG	UNP P63224
B	-17	SER	-	EXPRESSION TAG	UNP P63224
B	-16	SER	-	EXPRESSION TAG	UNP P63224
B	-15	HIS	-	EXPRESSION TAG	UNP P63224
B	-14	HIS	-	EXPRESSION TAG	UNP P63224
B	-13	HIS	-	EXPRESSION TAG	UNP P63224
B	-12	HIS	-	EXPRESSION TAG	UNP P63224
B	-11	HIS	-	EXPRESSION TAG	UNP P63224
B	-10	HIS	-	EXPRESSION TAG	UNP P63224
B	-9	SER	-	EXPRESSION TAG	UNP P63224
B	-8	SER	-	EXPRESSION TAG	UNP P63224
B	-7	GLY	-	EXPRESSION TAG	UNP P63224
B	-6	LEU	-	EXPRESSION TAG	UNP P63224
B	-5	VAL	-	EXPRESSION TAG	UNP P63224
B	-4	PRO	-	EXPRESSION TAG	UNP P63224
B	-3	ARG	-	EXPRESSION TAG	UNP P63224
B	-2	GLY	-	EXPRESSION TAG	UNP P63224
B	-1	SER	-	EXPRESSION TAG	UNP P63224
B	0	HIS	-	EXPRESSION TAG	UNP P63224
C	-19	MET	-	EXPRESSION TAG	UNP P63224
C	-18	GLY	-	EXPRESSION TAG	UNP P63224
C	-17	SER	-	EXPRESSION TAG	UNP P63224
C	-16	SER	-	EXPRESSION TAG	UNP P63224
C	-15	HIS	-	EXPRESSION TAG	UNP P63224
C	-14	HIS	-	EXPRESSION TAG	UNP P63224
C	-13	HIS	-	EXPRESSION TAG	UNP P63224
C	-12	HIS	-	EXPRESSION TAG	UNP P63224
C	-11	HIS	-	EXPRESSION TAG	UNP P63224
C	-10	HIS	-	EXPRESSION TAG	UNP P63224
C	-9	SER	-	EXPRESSION TAG	UNP P63224
C	-8	SER	-	EXPRESSION TAG	UNP P63224
C	-7	GLY	-	EXPRESSION TAG	UNP P63224
C	-6	LEU	-	EXPRESSION TAG	UNP P63224
C	-5	VAL	-	EXPRESSION TAG	UNP P63224
C	-4	PRO	-	EXPRESSION TAG	UNP P63224
C	-3	ARG	-	EXPRESSION TAG	UNP P63224
C	-2	GLY	-	EXPRESSION TAG	UNP P63224
C	-1	SER	-	EXPRESSION TAG	UNP P63224
C	0	HIS	-	EXPRESSION TAG	UNP P63224
D	-19	MET	-	EXPRESSION TAG	UNP P63224
D	-18	GLY	-	EXPRESSION TAG	UNP P63224
D	-17	SER	-	EXPRESSION TAG	UNP P63224

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	EXPRESSION TAG	UNP P63224
D	-15	HIS	-	EXPRESSION TAG	UNP P63224
D	-14	HIS	-	EXPRESSION TAG	UNP P63224
D	-13	HIS	-	EXPRESSION TAG	UNP P63224
D	-12	HIS	-	EXPRESSION TAG	UNP P63224
D	-11	HIS	-	EXPRESSION TAG	UNP P63224
D	-10	HIS	-	EXPRESSION TAG	UNP P63224
D	-9	SER	-	EXPRESSION TAG	UNP P63224
D	-8	SER	-	EXPRESSION TAG	UNP P63224
D	-7	GLY	-	EXPRESSION TAG	UNP P63224
D	-6	LEU	-	EXPRESSION TAG	UNP P63224
D	-5	VAL	-	EXPRESSION TAG	UNP P63224
D	-4	PRO	-	EXPRESSION TAG	UNP P63224
D	-3	ARG	-	EXPRESSION TAG	UNP P63224
D	-2	GLY	-	EXPRESSION TAG	UNP P63224
D	-1	SER	-	EXPRESSION TAG	UNP P63224
D	0	HIS	-	EXPRESSION TAG	UNP P63224

- Molecule 2 is D-ALTRO-HEPT-2-ULOSE 7-PHOSPHATE (three-letter code: I22) (formula:  $C_7H_{15}O_{10}P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			18	7	10	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	50	Total 50	O 50	0	0
3	B	52	Total 52	O 52	0	0
3	C	66	Total 66	O 66	0	0
3	D	43	Total 43	O 43	0	0



Chain D: 

MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	SER	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	HIS	M1	Y2	Q3	D4	I5	I6	R7	N8	E9	L10	M11	A14	E15	T16	L17	A18	L21	K22	D23	D24	H28	R32	A33	A34	F41	C50	G51	N52	G53	G54	S55	H56	C57	D58
A59	M60	E65	L66	R69	Y70	R71	E72	I82	S83	ASP	VAL	SER	ILE	SER	CYS	VAL	GLY	ASN	ASP	PHE	GLY	PHE	N98	D99	I100	R103	Y104	V105	E106	A107	V108	V114	L115	T120	N123	S124	V127	I128	K129	A130	I131	A134	V141	I142	T143	L144	K147						
D148	G149	G150	K151	M152	T155	A156	D157	I158	R161	V162	F163	H164	F165	G166	Y167	A168	D169	R170	I171	Q172	E173	I174	H175	I176	K177	V178	I179	H180	I181	L182	I183	Q184	L185	I186	E187	K188	E189	M190	V191	K192													



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	73.05Å 76.54Å 78.32Å 90.00° 106.13° 90.00°	Depositor
Resolution (Å)	25.00 – 2.80 47.39 – 2.79	Depositor EDS
% Data completeness (in resolution range)	100.0 (25.00-2.80) 98.5 (47.39-2.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.71 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.203 , 0.257 0.194 , 0.245	Depositor DCC
$R_{free}$ test set	1499 reflections (7.88%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.0	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 32.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 20523 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5665	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.45% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: I22

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	1.73	16/1382 (1.2%)	1.46	13/1856 (0.7%)
1	B	1.76	18/1374 (1.3%)	1.43	12/1845 (0.7%)
1	C	1.78	17/1374 (1.2%)	1.47	14/1845 (0.8%)
1	D	1.73	17/1374 (1.2%)	1.49	16/1845 (0.9%)
All	All	1.75	68/5504 (1.2%)	1.46	55/7391 (0.7%)

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	63	ALA	CA-CB	-10.38	1.30	1.52
1	B	136	GLU	CG-CD	8.52	1.64	1.51
1	A	117	GLY	N-CA	7.75	1.57	1.46
1	A	165	PHE	CE1-CZ	7.52	1.51	1.37
1	C	140	LYS	CE-NZ	7.50	1.67	1.49
1	A	65	GLU	CD-OE1	7.46	1.33	1.25
1	C	83	SER	C-O	7.38	1.37	1.23
1	D	14	ALA	CA-CB	-7.24	1.37	1.52
1	D	50	CYS	CB-SG	7.19	1.94	1.82
1	B	173	GLU	CD-OE1	7.12	1.33	1.25
1	C	159	GLU	CD-OE2	6.87	1.33	1.25
1	D	104	TYR	CD2-CE2	6.78	1.49	1.39
1	C	65	GLU	CD-OE1	6.78	1.33	1.25
1	A	178	VAL	C-O	6.60	1.35	1.23
1	B	165	PHE	CE1-CZ	6.51	1.49	1.37
1	C	49	SER	N-CA	-6.47	1.33	1.46
1	C	167	TYR	CG-CD2	6.46	1.47	1.39
1	C	147	LYS	CE-NZ	6.44	1.65	1.49
1	D	178	VAL	CB-CG2	6.33	1.66	1.52
1	D	141	VAL	CB-CG1	6.26	1.66	1.52
1	A	13	ALA	CA-CB	6.21	1.65	1.52
1	B	59	ALA	CA-CB	-6.14	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	136	GLU	CD-OE2	6.05	1.32	1.25
1	C	15	GLU	CB-CG	6.03	1.63	1.52
1	B	167	TYR	CD2-CE2	5.94	1.48	1.39
1	D	191	VAL	CB-CG1	5.92	1.65	1.52
1	B	133	ALA	CA-CB	-5.92	1.40	1.52
1	D	106	GLU	CD-OE2	-5.87	1.19	1.25
1	A	159	GLU	CD-OE2	5.85	1.32	1.25
1	B	77	TYR	CG-CD2	-5.79	1.31	1.39
1	D	15	GLU	C-O	5.78	1.34	1.23
1	D	167	TYR	CG-CD2	5.78	1.46	1.39
1	B	72	GLU	CG-CD	5.77	1.60	1.51
1	B	176	ILE	N-CA	-5.76	1.34	1.46
1	A	57	CYS	CB-SG	5.71	1.92	1.82
1	D	9	GLU	CB-CG	5.69	1.62	1.52
1	B	184	GLN	CG-CD	5.55	1.63	1.51
1	B	57	CYS	CB-SG	5.55	1.91	1.82
1	C	127	VAL	CB-CG1	5.53	1.64	1.52
1	B	130	ALA	CA-CB	-5.50	1.41	1.52
1	A	129	LYS	CE-NZ	5.46	1.62	1.49
1	B	127	VAL	CB-CG1	-5.45	1.41	1.52
1	C	43	ALA	CA-CB	5.44	1.63	1.52
1	C	174	ILE	N-CA	-5.43	1.35	1.46
1	D	106	GLU	CB-CG	-5.42	1.41	1.52
1	C	191	VAL	CB-CG1	5.42	1.64	1.52
1	C	159	GLU	CD-OE1	5.42	1.31	1.25
1	D	15	GLU	CG-CD	5.41	1.60	1.51
1	D	52	ASN	CB-CG	5.32	1.63	1.51
1	A	159	GLU	CD-OE1	5.24	1.31	1.25
1	D	187	GLU	CG-CD	5.21	1.59	1.51
1	D	167	TYR	CG-CD1	5.20	1.46	1.39
1	B	104	TYR	CD1-CE1	-5.20	1.31	1.39
1	B	136	GLU	CB-CG	5.19	1.62	1.52
1	B	167	TYR	CZ-OH	-5.18	1.29	1.37
1	A	191	VAL	CA-CB	5.17	1.65	1.54
1	A	82	ILE	CA-CB	-5.15	1.43	1.54
1	A	22	LYS	CB-CG	5.14	1.66	1.52
1	D	11	ASN	C-O	5.14	1.33	1.23
1	C	173	GLU	CD-OE2	5.13	1.31	1.25
1	A	134	ALA	CA-CB	-5.10	1.41	1.52
1	C	70	TYR	CD1-CE1	-5.07	1.31	1.39
1	B	12	GLU	CG-CD	5.05	1.59	1.51
1	A	124	SER	CB-OG	5.04	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	98	ASN	CB-CG	5.03	1.62	1.51
1	C	176	ILE	CB-CG2	-5.03	1.37	1.52
1	D	65	GLU	CD-OE2	5.02	1.31	1.25
1	A	165	PHE	CD2-CE2	5.01	1.49	1.39

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	103	ARG	NE-CZ-NH1	11.08	125.84	120.30
1	A	161	ARG	NE-CZ-NH1	-10.47	115.06	120.30
1	C	103	ARG	NE-CZ-NH1	9.83	125.22	120.30
1	C	60	MET	CG-SD-CE	9.47	115.35	100.20
1	C	39	ASP	CB-CG-OD1	9.26	126.64	118.30
1	A	58	ASP	CB-CG-OD1	9.26	126.64	118.30
1	A	169	ASP	CB-CG-OD1	-9.25	109.98	118.30
1	C	5	LEU	CB-CG-CD1	-8.86	95.94	111.00
1	D	169	ASP	CB-CG-OD1	-8.65	110.52	118.30
1	A	161	ARG	NE-CZ-NH2	8.64	124.62	120.30
1	D	69	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	C	135	ARG	NE-CZ-NH1	-8.16	116.22	120.30
1	B	32	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	D	60	MET	CG-SD-CE	6.92	111.27	100.20
1	B	182	LEU	CB-CG-CD2	-6.88	99.30	111.00
1	A	103	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	C	151	LYS	CD-CE-NZ	-6.70	96.29	111.70
1	D	57	CYS	CA-CB-SG	-6.63	102.07	114.00
1	D	188	LYS	CD-CE-NZ	-6.50	96.74	111.70
1	D	5	LEU	CB-CG-CD1	-6.46	100.03	111.00
1	C	169	ASP	CB-CG-OD1	-6.42	112.52	118.30
1	D	169	ASP	CB-CG-OD2	6.40	124.06	118.30
1	B	103	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	21	LEU	CB-CG-CD2	-6.37	100.17	111.00
1	A	82	ILE	CG1-CB-CG2	-6.30	97.53	111.40
1	C	169	ASP	CB-CG-OD2	6.21	123.89	118.30
1	C	78	PRO	N-CD-CG	-6.07	94.09	103.20
1	A	23	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	C	57	CYS	CA-CB-SG	-6.00	103.20	114.00
1	A	103	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	B	158	ILE	CG1-CB-CG2	-5.93	98.35	111.40
1	B	4	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	D	106	GLU	CG-CD-OE2	-5.88	106.55	118.30
1	B	39	ASP	CB-CG-OD2	-5.76	113.11	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	100	ILE	CG1-CB-CG2	-5.70	98.86	111.40
1	D	161	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	C	61	HIS	N-CA-CB	5.67	120.81	110.60
1	A	39	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	A	144	LEU	CB-CG-CD1	-5.63	101.43	111.00
1	B	103	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	66	LEU	CB-CG-CD1	-5.58	101.52	111.00
1	D	170	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	D	106	GLU	CG-CD-OE1	5.41	129.11	118.30
1	C	16	THR	OG1-CB-CG2	-5.40	97.57	110.00
1	D	50	CYS	CA-CB-SG	-5.39	104.30	114.00
1	B	191	VAL	CG1-CB-CG2	-5.36	102.33	110.90
1	A	123	ASN	N-CA-C	5.28	125.25	111.00
1	D	157	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	B	23	ASP	CB-CG-OD1	5.20	122.98	118.30
1	D	148	ASP	CB-CG-OD1	-5.18	113.64	118.30
1	B	71	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	169	ASP	CB-CG-OD2	5.16	122.95	118.30
1	C	159	GLU	OE1-CD-OE2	5.12	129.45	123.30
1	A	84	ASP	CB-CG-OD2	5.09	122.88	118.30
1	C	23	ASP	CB-CG-OD2	-5.08	113.73	118.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1365	0	1375	116	0
1	B	1357	0	1371	88	0
1	C	1357	0	1371	75	0
1	D	1357	0	1371	93	0
2	B	18	0	13	14	0
3	A	50	0	0	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	52	0	0	10	0
3	C	66	0	0	4	0
3	D	43	0	0	1	0
All	All	5665	0	5501	346	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 32.

All (346) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:142:ILE:CD1	1:D:142:ILE:CG1	1.79	1.52
1:C:140:LYS:NZ	1:C:140:LYS:CE	1.67	1.52
1:A:83:SER:HA	3:A:200:HOH:O	1.44	1.15
1:C:2:TYR:O	1:C:6:ILE:HD13	1.49	1.11
1:A:172:GLN:C	1:A:172:GLN:HE21	1.55	1.06
1:B:28:HIS:HB3	3:B:933:HOH:O	1.55	1.05
1:B:169:ASP:HB2	3:B:926:HOH:O	1.57	1.04
1:A:163:PRO:HD3	3:A:241:HOH:O	1.56	1.02
3:A:196:HOH:O	1:D:3:GLN:HG3	1.59	1.00
1:B:54:GLY:HA3	2:B:900:I22:O5	1.62	1.00
1:A:103:ARG:HG2	1:A:103:ARG:HH11	1.27	0.99
1:D:3:GLN:HG2	1:D:7:ARG:HH12	1.26	0.97
1:C:22:LYS:HG2	1:C:23:ASP:N	1.80	0.95
1:B:24:ASP:O	1:B:28:HIS:HD2	1.50	0.95
1:D:3:GLN:HG2	1:D:7:ARG:NH1	1.83	0.91
2:B:900:I22:O1	2:B:900:I22:H5	1.69	0.90
1:B:57:CYS:HG	1:C:57:CYS:HG	0.94	0.89
1:A:172:GLN:C	1:A:172:GLN:NE2	2.26	0.89
1:D:3:GLN:CG	1:D:7:ARG:HH12	1.86	0.88
1:A:31:GLN:HE22	1:D:1:MET:HA	1.38	0.87
2:B:900:I22:O1	2:B:900:I22:C5	2.22	0.87
1:A:127:VAL:O	1:A:131:ILE:CG1	2.25	0.85
1:B:70:TYR:CE2	1:B:190:MET:HG3	2.13	0.83
1:A:22:LYS:HG2	1:A:23:ASP:N	1.93	0.83
1:C:22:LYS:HG2	1:C:23:ASP:H	1.42	0.82
1:B:131:ILE:HG23	1:B:141:VAL:HG11	1.58	0.82
1:B:131:ILE:HD13	1:B:141:VAL:CG1	2.10	0.82
1:D:58:ASP:HB3	1:D:179:ILE:CD1	2.10	0.82
1:D:98:ASN:HD22	1:D:129:LYS:HZ3	1.25	0.82
1:C:2:TYR:O	1:C:6:ILE:CD1	2.28	0.82
1:A:28:HIS:HD2	3:A:196:HOH:O	1.62	0.81
1:A:172:GLN:O	1:A:175:HIS:HB2	1.81	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:98:ASN:HB3	1:D:129:LYS:HZ2	1.46	0.81
1:A:28:HIS:CD2	3:A:196:HOH:O	2.34	0.80
1:A:127:VAL:O	1:A:131:ILE:HG12	1.82	0.80
1:B:131:ILE:HD13	1:B:141:VAL:HG11	1.64	0.80
1:D:98:ASN:ND2	1:D:129:LYS:HZ3	1.80	0.80
1:C:6:ILE:N	1:C:6:ILE:HD12	1.96	0.79
1:B:56:HIS:CD2	3:B:938:HOH:O	2.33	0.79
1:B:162:VAL:HB	1:B:171:ILE:HG23	1.66	0.78
1:B:24:ASP:O	1:B:28:HIS:CD2	2.38	0.77
1:A:98:ASN:CB	3:A:220:HOH:O	2.33	0.76
1:A:177:LYS:HZ1	1:D:177:LYS:HZ1	1.33	0.76
1:C:21:LEU:O	1:C:21:LEU:HD12	1.85	0.76
2:B:900:I22:C1	2:B:900:I22:O5	2.34	0.76
1:C:6:ILE:H	1:C:6:ILE:HD12	1.49	0.75
1:D:147:LYS:O	1:D:161:ARG:HD3	1.85	0.75
1:B:46:LYS:O	1:B:113:ASP:HB3	1.86	0.75
1:B:144:LEU:HB3	1:B:175:HIS:CD2	2.21	0.75
1:D:172:GLN:C	1:D:172:GLN:HE21	1.90	0.75
1:B:177:LYS:NZ	1:C:177:LYS:HZ1	1.85	0.74
1:D:124:SER:O	1:D:128:ILE:HD12	1.86	0.74
1:A:98:ASN:HB3	3:A:220:HOH:O	1.86	0.74
1:D:157:ASP:O	1:D:158:ILE:HG13	1.88	0.74
1:B:7:ARG:NH2	1:C:24:ASP:OD2	2.22	0.73
1:D:98:ASN:HB3	1:D:129:LYS:NZ	2.04	0.72
1:A:99:ASP:CB	3:A:204:HOH:O	2.37	0.72
1:A:127:VAL:O	1:A:131:ILE:HG13	1.87	0.72
1:C:22:LYS:CG	1:C:23:ASP:N	2.51	0.71
1:D:127:VAL:O	1:D:131:ILE:HG13	1.91	0.70
1:D:22:LYS:HG2	1:D:23:ASP:N	2.06	0.70
2:B:900:I22:H3	1:C:180:HIS:NE2	2.06	0.70
1:A:71:ARG:HG3	1:A:72:GLU:N	2.07	0.69
1:D:98:ASN:CB	1:D:129:LYS:NZ	2.55	0.69
1:D:174:ILE:O	1:D:178:VAL:HG23	1.92	0.69
1:A:38:ALA:HA	1:A:190:MET:CE	2.23	0.69
1:B:2:TYR:HA	3:B:940:HOH:O	1.93	0.69
1:D:82:ILE:HG23	1:D:104:TYR:CD2	2.27	0.69
1:C:176:ILE:HA	1:C:179:ILE:HG13	1.74	0.69
1:C:6:ILE:H	1:C:6:ILE:CD1	2.06	0.69
1:B:103:ARG:HH11	1:B:103:ARG:HG2	1.56	0.69
1:A:177:LYS:NZ	1:D:177:LYS:NZ	2.42	0.68
1:A:31:GLN:NE2	1:D:1:MET:HA	2.08	0.68
1:A:177:LYS:NZ	1:D:177:LYS:HZ1	1.91	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:182:LEU:O	1:B:186:ILE:HG13	1.93	0.67
1:B:26:ASN:O	1:B:30:ILE:HG13	1.95	0.67
1:A:22:LYS:HG2	1:A:23:ASP:H	1.59	0.67
1:A:131:ILE:HG23	1:A:141:VAL:HG11	1.75	0.67
1:D:3:GLN:CD	1:D:7:ARG:HH12	1.98	0.67
1:B:177:LYS:NZ	1:C:177:LYS:NZ	2.42	0.67
1:A:103:ARG:CG	1:A:103:ARG:HH11	2.07	0.66
1:A:103:ARG:HG2	1:A:103:ARG:NH1	2.04	0.66
1:B:8:ASN:ND2	3:B:913:HOH:O	2.30	0.65
1:D:191:VAL:O	1:D:191:VAL:HG23	1.97	0.65
1:C:175:HIS:O	1:C:179:ILE:HG12	1.97	0.64
1:C:15:GLU:O	1:C:18:ALA:HB3	1.97	0.64
1:C:122:GLY:O	1:C:152:MET:HG3	1.98	0.64
1:A:21:LEU:O	1:A:21:LEU:HD12	1.98	0.64
1:D:142:ILE:CD1	1:D:142:ILE:CB	2.72	0.64
1:D:98:ASN:HD22	1:D:129:LYS:NZ	1.96	0.64
1:B:191:VAL:CG2	1:B:191:VAL:O	2.46	0.64
1:D:28:HIS:O	1:D:32:ARG:HG3	1.97	0.64
1:B:191:VAL:HG23	1:B:191:VAL:O	1.98	0.63
1:B:54:GLY:HA3	2:B:900:I22:HO5	1.60	0.63
1:A:175:HIS:O	1:A:179:ILE:HG13	1.99	0.62
1:A:57:CYS:O	1:A:58:ASP:C	2.34	0.62
1:D:98:ASN:ND2	1:D:129:LYS:NZ	2.46	0.62
1:D:98:ASN:C	1:D:129:LYS:HZ1	2.02	0.62
1:A:162:VAL:HG12	1:A:162:VAL:O	2.00	0.62
1:A:37:LEU:O	1:A:40:SER:HB2	1.99	0.62
1:A:36:LEU:O	1:A:36:LEU:HD12	2.00	0.62
1:A:169:ASP:OD1	1:A:169:ASP:N	2.26	0.62
1:A:177:LYS:HZ1	1:D:177:LYS:NZ	1.98	0.62
1:C:124:SER:O	1:C:128:ILE:HD12	1.99	0.62
1:C:191:VAL:HG23	1:C:191:VAL:O	1.98	0.61
1:A:17:LEU:HD12	1:A:17:LEU:O	2.01	0.61
1:B:184:GLN:NE2	3:B:909:HOH:O	2.34	0.61
1:A:5:LEU:O	1:A:8:ASN:HB3	2.01	0.60
1:D:147:LYS:HA	1:D:164:HIS:O	2.00	0.60
1:C:123:ASN:OD1	1:C:150:GLY:HA3	2.02	0.60
1:C:167:TYR:CD2	1:C:168:ALA:N	2.70	0.60
1:A:101:PHE:CD1	1:A:126:ASN:HB2	2.36	0.60
2:B:900:I22:H12	2:B:900:I22:O5	2.01	0.60
1:D:144:LEU:O	1:D:175:HIS:CE1	2.55	0.60
1:B:19:ASN:HA	1:B:22:LYS:HD2	1.84	0.60
1:D:98:ASN:N	3:D:211:HOH:O	2.34	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:98:ASN:HB2	3:A:220:HOH:O	1.98	0.59
1:A:22:LYS:NZ	3:A:212:HOH:O	2.34	0.59
1:B:37:LEU:HD13	1:B:62:PHE:HZ	1.65	0.59
1:B:177:LYS:HZ1	1:C:177:LYS:HZ1	1.49	0.59
1:D:98:ASN:C	1:D:129:LYS:NZ	2.56	0.59
1:A:172:GLN:NE2	1:A:173:GLU:N	2.51	0.59
1:A:22:LYS:CG	1:A:23:ASP:N	2.63	0.59
1:A:162:VAL:HB	1:A:171:ILE:HG23	1.85	0.58
1:A:164:HIS:CD2	1:A:166:GLY:H	2.21	0.57
1:A:147:LYS:HG2	1:A:165:PHE:HA	1.87	0.57
1:C:5:LEU:O	1:C:8:ASN:HB2	2.04	0.57
1:A:49:SER:OG	1:A:59:ALA:HB1	2.03	0.57
1:D:15:GLU:O	1:D:18:ALA:HB3	2.03	0.57
1:D:50:CYS:HB3	1:D:82:ILE:HG13	1.86	0.57
1:C:140:LYS:CD	1:C:140:LYS:NZ	2.62	0.57
1:C:159:GLU:OE1	1:C:161:ARG:NE	2.33	0.57
1:A:24:ASP:OD2	1:D:7:ARG:NH2	2.38	0.57
1:C:71:ARG:HG3	1:C:72:GLU:N	2.20	0.57
1:C:21:LEU:C	1:C:21:LEU:HD12	2.25	0.56
2:B:900:I22:C1	2:B:900:I22:C5	2.84	0.56
1:B:24:ASP:HB3	1:B:28:HIS:NE2	2.21	0.56
1:D:184:GLN:O	1:D:187:GLU:HB3	2.06	0.56
1:C:5:LEU:O	1:C:9:GLU:HG2	2.06	0.56
1:B:162:VAL:CB	1:B:171:ILE:HG23	2.33	0.55
1:B:173:GLU:O	1:B:176:ILE:HG22	2.05	0.55
1:B:177:LYS:HZ3	1:C:177:LYS:NZ	2.04	0.55
1:A:52:ASN:O	1:A:55:SER:HB2	2.06	0.55
1:B:7:ARG:O	1:B:11:ASN:HB2	2.06	0.55
1:D:164:HIS:CE1	1:D:166:GLY:H	2.25	0.55
1:C:16:THR:HG23	3:C:217:HOH:O	2.06	0.55
1:D:103:ARG:HA	1:D:106:GLU:OE1	2.07	0.55
1:A:103:ARG:NH1	1:A:103:ARG:CG	2.67	0.55
1:B:103:ARG:NH1	1:B:103:ARG:HG2	2.21	0.55
1:B:177:LYS:HZ1	1:C:177:LYS:NZ	2.04	0.54
1:D:148:ASP:N	1:D:148:ASP:OD1	2.39	0.54
1:B:3:GLN:HB3	3:B:907:HOH:O	2.06	0.54
1:B:127:VAL:O	1:B:131:ILE:HG13	2.07	0.54
1:D:17:LEU:HD12	1:D:17:LEU:O	2.08	0.54
1:B:120:THR:O	1:B:146:GLY:HA3	2.08	0.53
1:B:54:GLY:HA3	2:B:900:I22:H12	1.89	0.53
1:B:104:TYR:O	1:B:105:VAL:C	2.45	0.53
1:A:126:ASN:H	1:A:126:ASN:ND2	2.06	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:99:ASP:OD1	1:B:99:ASP:N	2.42	0.53
1:A:23:ASP:C	1:A:23:ASP:OD1	2.47	0.53
1:A:10:LEU:CD2	1:D:181:ILE:HD11	2.39	0.53
1:B:58:ASP:HB3	1:B:179:ILE:CD1	2.39	0.53
1:B:146:GLY:HA3	1:B:171:ILE:HD13	1.91	0.53
1:C:5:LEU:HD23	1:C:5:LEU:O	2.09	0.52
1:C:2:TYR:HA	3:C:202:HOH:O	2.09	0.52
1:B:58:ASP:HB3	1:B:179:ILE:HD12	1.90	0.52
1:A:57:CYS:O	1:A:60:MET:N	2.41	0.52
1:A:10:LEU:O	1:A:13:ALA:HB3	2.09	0.52
1:D:120:THR:HG21	1:D:168:ALA:HB1	1.91	0.52
1:A:10:LEU:HD21	1:D:181:ILE:CD1	2.38	0.52
1:D:21:LEU:O	1:D:21:LEU:HD12	2.09	0.52
1:B:4:ASP:O	1:B:8:ASN:HB2	2.10	0.52
1:C:3:GLN:HB3	3:C:210:HOH:O	2.08	0.52
1:A:10:LEU:HD23	1:D:181:ILE:HD11	1.91	0.52
1:A:52:ASN:ND2	1:A:126:ASN:OD1	2.34	0.52
1:B:147:LYS:O	1:B:161:ARG:HD3	2.10	0.52
1:B:176:ILE:HG23	1:B:177:LYS:N	2.25	0.52
1:C:103:ARG:HH11	1:C:103:ARG:HG2	1.76	0.51
1:C:76:GLY:HA2	1:D:103:ARG:O	2.11	0.51
1:C:162:VAL:HB	1:C:171:ILE:HG23	1.91	0.51
1:A:162:VAL:CB	1:A:171:ILE:HG23	2.41	0.51
1:A:99:ASP:HB3	3:A:204:HOH:O	2.05	0.51
1:A:108:VAL:HG12	1:B:108:VAL:HB	1.92	0.51
1:A:171:ILE:O	1:A:172:GLN:C	2.48	0.51
1:A:84:ASP:C	1:A:84:ASP:OD1	2.49	0.51
1:A:10:LEU:CD2	1:D:181:ILE:CD1	2.89	0.51
1:B:190:MET:C	1:B:192:LYS:H	2.13	0.51
1:B:71:ARG:HG3	1:B:72:GLU:N	2.24	0.51
1:B:98:ASN:HD22	1:B:129:LYS:NZ	2.09	0.51
1:A:177:LYS:HZ3	1:D:177:LYS:NZ	2.09	0.51
1:B:69:ARG:HB2	1:B:70:TYR:CD1	2.45	0.51
1:D:17:LEU:HD22	1:D:177:LYS:HE2	1.93	0.51
1:D:123:ASN:OD1	1:D:151:LYS:HG3	2.11	0.51
1:A:38:ALA:CA	1:A:190:MET:HE1	2.41	0.50
1:A:172:GLN:O	1:A:175:HIS:N	2.44	0.50
1:A:168:ALA:O	1:A:171:ILE:N	2.44	0.50
1:D:58:ASP:HB3	1:D:179:ILE:HD13	1.92	0.50
1:A:1:MET:HA	1:A:3:GLN:HG2	1.94	0.50
1:D:98:ASN:O	1:D:129:LYS:NZ	2.45	0.50
1:C:32:ARG:HH11	1:C:32:ARG:HG3	1.77	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:38:ALA:HB1	1:A:190:MET:HE1	1.93	0.50
1:D:152:MET:O	1:D:155:THR:OG1	2.27	0.49
1:B:22:LYS:HG2	1:B:23:ASP:N	2.28	0.49
1:C:71:ARG:HG3	1:C:72:GLU:H	1.76	0.49
1:C:46:LYS:NZ	1:C:113:ASP:OD2	2.31	0.49
1:D:98:ASN:CB	1:D:129:LYS:HZ1	2.26	0.49
1:D:150:GLY:C	1:D:152:MET:H	2.16	0.48
1:D:162:VAL:HB	1:D:171:ILE:HG23	1.95	0.48
1:A:41:PHE:O	1:A:44:GLY:N	2.44	0.48
1:A:182:LEU:O	1:A:186:ILE:HG13	2.14	0.48
1:B:5:LEU:HD13	1:C:185:LEU:CD2	2.44	0.48
1:D:98:ASN:CA	1:D:129:LYS:HZ1	2.25	0.48
1:B:144:LEU:HB3	1:B:175:HIS:NE2	2.29	0.48
1:C:152:MET:O	1:C:155:THR:OG1	2.28	0.48
1:A:110:ARG:HB2	1:A:113:ASP:OD2	2.13	0.48
1:D:5:LEU:O	1:D:8:ASN:HB2	2.14	0.48
1:B:54:GLY:N	1:C:61:HIS:CE1	2.82	0.48
1:B:61:HIS:O	1:B:62:PHE:C	2.49	0.48
1:B:67:THR:HA	1:B:78:PRO:HD2	1.96	0.48
1:D:99:ASP:OD2	1:D:103:ARG:NE	2.46	0.48
1:A:38:ALA:CA	1:A:190:MET:CE	2.92	0.47
1:D:71:ARG:HG3	1:D:72:GLU:N	2.29	0.47
1:A:107:ALA:C	1:A:108:VAL:CG1	2.83	0.47
1:A:177:LYS:O	1:A:178:VAL:C	2.52	0.47
1:A:41:PHE:HB2	1:A:190:MET:HE3	1.97	0.47
1:A:49:SER:O	1:A:82:ILE:HG13	2.14	0.47
1:D:52:ASN:O	1:D:53:GLY:C	2.52	0.47
1:B:24:ASP:OD2	1:C:7:ARG:NH2	2.48	0.47
2:B:900:I22:H3	1:C:180:HIS:CD2	2.49	0.46
1:C:12:GLU:O	1:C:16:THR:OG1	2.33	0.46
1:D:172:GLN:O	1:D:175:HIS:HB2	2.15	0.46
1:A:71:ARG:CG	1:A:72:GLU:N	2.76	0.46
1:A:28:HIS:O	1:A:31:GLN:N	2.48	0.46
1:D:98:ASN:O	1:D:129:LYS:CE	2.64	0.46
1:A:46:LYS:N	1:A:113:ASP:OD1	2.36	0.46
1:A:70:TYR:CE2	1:A:190:MET:HG3	2.50	0.46
1:C:5:LEU:CD2	1:C:5:LEU:C	2.83	0.46
1:B:147:LYS:HA	1:B:164:HIS:O	2.15	0.46
1:A:7:ARG:NH2	1:D:24:ASP:OD2	2.48	0.46
1:A:58:ASP:HB3	1:A:179:ILE:CD1	2.45	0.46
1:A:104:TYR:O	1:A:105:VAL:C	2.54	0.46
1:B:56:HIS:HD2	3:B:938:HOH:O	1.87	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:6:ILE:HD13	1:D:6:ILE:HG21	1.51	0.46
1:C:176:ILE:HG23	1:C:177:LYS:N	2.30	0.46
1:B:172:GLN:O	1:B:175:HIS:HB2	2.16	0.46
2:B:900:I22:C2	1:C:61:HIS:HD1	2.28	0.45
1:D:58:ASP:HB3	1:D:179:ILE:HD12	1.95	0.45
1:A:110:ARG:O	1:A:113:ASP:HB2	2.16	0.45
1:C:167:TYR:HD2	1:C:168:ALA:H	1.59	0.45
1:D:170:ARG:O	1:D:174:ILE:HG12	2.16	0.45
1:A:143:THR:O	1:A:144:LEU:HD23	2.17	0.45
1:B:103:ARG:HA	1:B:106:GLU:OE1	2.17	0.45
1:A:114:VAL:HG12	1:A:115:LEU:N	2.31	0.45
1:B:21:LEU:HD12	1:B:21:LEU:O	2.16	0.45
1:D:100:ILE:HD13	1:D:100:ILE:HG21	1.48	0.45
1:A:162:VAL:O	1:A:164:HIS:N	2.44	0.45
1:B:2:TYR:OH	1:C:189:GLU:HG2	2.17	0.45
1:B:1:MET:N	3:B:906:HOH:O	2.50	0.45
1:C:116:LEU:HA	1:C:142:ILE:O	2.17	0.45
1:C:32:ARG:NH1	1:C:32:ARG:HG3	2.31	0.45
1:C:10:LEU:HA	1:C:10:LEU:HD23	1.61	0.44
1:A:29:ALA:HB1	1:A:160:ILE:HG12	1.99	0.44
1:D:114:VAL:HG12	1:D:115:LEU:N	2.30	0.44
1:C:99:ASP:N	1:C:99:ASP:OD1	2.48	0.44
1:D:4:ASP:C	1:D:8:ASN:HD22	2.18	0.44
1:B:124:SER:O	1:B:128:ILE:HG13	2.17	0.44
1:B:47:VAL:HG12	1:B:78:PRO:O	2.17	0.44
1:A:21:LEU:O	1:A:27:ILE:HD11	2.17	0.44
1:B:100:ILE:HG23	1:B:101:PHE:CD2	2.53	0.44
1:A:38:ALA:CB	1:A:190:MET:HE1	2.48	0.44
1:A:184:GLN:O	1:A:185:LEU:C	2.54	0.44
1:D:157:ASP:C	1:D:158:ILE:HG13	2.38	0.44
1:B:7:ARG:HG3	1:B:7:ARG:HH11	1.82	0.44
1:C:38:ALA:O	1:C:42:LYS:HG3	2.18	0.44
1:D:131:ILE:O	1:D:134:ALA:HB3	2.17	0.43
1:A:107:ALA:C	1:A:108:VAL:HG13	2.37	0.43
1:A:57:CYS:SG	1:D:57:CYS:HA	2.58	0.43
1:A:60:MET:O	1:A:63:ALA:N	2.51	0.43
1:D:129:LYS:HB2	1:D:129:LYS:HE2	1.56	0.43
1:A:168:ALA:O	1:A:169:ASP:C	2.56	0.43
1:A:110:ARG:NH2	1:B:109:GLY:O	2.51	0.43
1:C:37:LEU:HA	1:C:37:LEU:HD23	1.76	0.43
1:C:50:CYS:HA	3:C:204:HOH:O	2.18	0.43
1:B:57:CYS:SG	1:C:57:CYS:HA	2.59	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:176:ILE:CG2	1:B:177:LYS:N	2.81	0.43
2:B:900:I22:O1	2:B:900:I22:O5	2.37	0.43
1:A:127:VAL:HG12	1:A:127:VAL:O	2.18	0.43
1:C:5:LEU:HD23	1:C:5:LEU:C	2.39	0.43
1:A:20:PHE:HZ	1:A:30:ILE:HD11	1.83	0.43
1:C:147:LYS:HA	1:C:164:HIS:O	2.18	0.43
1:A:58:ASP:HB3	1:A:179:ILE:HD11	2.01	0.42
1:D:66:LEU:HD21	1:D:183:ILE:CG1	2.48	0.42
1:D:70:TYR:CE2	1:D:190:MET:HG3	2.54	0.42
2:B:900:I22:O5	2:B:900:I22:C2	2.67	0.42
1:B:98:ASN:HD22	1:B:129:LYS:HZ2	1.66	0.42
1:C:100:ILE:HG21	1:C:100:ILE:HD13	1.64	0.42
1:A:77:TYR:HA	1:A:78:PRO:HD3	1.85	0.42
1:A:114:VAL:O	1:A:139:MET:CE	2.67	0.42
1:C:66:LEU:CD2	1:C:183:ILE:HG12	2.49	0.42
1:C:186:ILE:HD13	1:C:186:ILE:HG21	1.71	0.42
1:B:186:ILE:HD13	1:B:186:ILE:HG21	1.65	0.42
1:A:164:HIS:HB3	1:A:171:ILE:HG12	2.01	0.42
1:D:82:ILE:HG23	1:D:104:TYR:CG	2.55	0.42
1:D:41:PHE:N	1:D:41:PHE:CD1	2.86	0.42
1:A:2:TYR:OH	1:D:189:GLU:HG2	2.19	0.42
1:D:98:ASN:O	1:D:129:LYS:HE3	2.20	0.42
1:B:17:LEU:HD22	1:B:177:LYS:HE2	2.02	0.42
1:B:28:HIS:CB	3:B:933:HOH:O	2.36	0.41
1:B:54:GLY:CA	2:B:900:I22:O5	2.50	0.41
1:A:137:LYS:HD3	1:A:137:LYS:HA	1.85	0.41
1:C:184:GLN:O	1:C:187:GLU:HB3	2.20	0.41
1:A:177:LYS:NZ	1:D:177:LYS:HZ3	2.18	0.41
1:D:34:ALA:CB	1:D:185:LEU:HB2	2.50	0.41
1:B:123:ASN:OD1	1:B:150:GLY:HA3	2.20	0.41
1:A:26:ASN:O	1:A:27:ILE:C	2.59	0.41
1:A:116:LEU:HA	1:A:142:ILE:O	2.20	0.41
1:D:169:ASP:N	1:D:169:ASP:OD1	2.54	0.41
1:A:118:ILE:HD13	1:A:118:ILE:HG21	1.75	0.41
1:A:165:PHE:N	3:A:199:HOH:O	2.54	0.41
1:D:144:LEU:O	1:D:175:HIS:HE1	2.02	0.41
1:D:162:VAL:HG21	1:D:174:ILE:HB	2.02	0.41
1:A:76:GLY:O	1:B:103:ARG:NH1	2.54	0.41
1:B:12:GLU:OE2	1:B:164:HIS:HE1	2.04	0.41
1:A:29:ALA:CB	1:A:160:ILE:HG12	2.50	0.41
1:A:131:ILE:CG2	1:A:141:VAL:HG11	2.46	0.41
1:A:19:ASN:HA	1:A:22:LYS:HD2	2.02	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:69:ARG:HB2	1:B:70:TYR:CE1	2.56	0.41
1:A:107:ALA:CB	1:A:108:VAL:HG13	2.51	0.41
1:B:118:ILE:HG21	1:B:118:ILE:HD13	1.89	0.41
1:B:152:MET:O	1:B:155:THR:OG1	2.35	0.41
1:C:23:ASP:OD1	1:C:23:ASP:C	2.60	0.40
1:D:147:LYS:CA	1:D:164:HIS:O	2.69	0.40
1:A:99:ASP:N	1:A:99:ASP:OD1	2.41	0.40
1:D:191:VAL:CG2	1:D:191:VAL:O	2.68	0.40
1:D:66:LEU:HD21	1:D:183:ILE:HG13	2.02	0.40
1:B:60:MET:HB3	1:B:60:MET:HE3	1.92	0.40
1:B:28:HIS:CD2	1:B:28:HIS:N	2.89	0.40
1:C:174:ILE:HD12	1:C:174:ILE:HG23	1.89	0.40
1:B:31:GLN:HE22	1:C:1:MET:HA	1.86	0.40
1:C:103:ARG:NH1	1:C:103:ARG:HG2	2.36	0.40
1:C:182:LEU:O	1:C:186:ILE:HG13	2.21	0.40
1:C:63:ALA:HA	1:C:79:ALA:HB1	2.03	0.40
1:D:17:LEU:C	1:D:17:LEU:HD12	2.41	0.40
1:C:99:ASP:OD2	1:C:103:ARG:NE	2.54	0.40
1:C:66:LEU:HD21	1:C:183:ILE:HG12	2.04	0.40
1:A:148:ASP:O	1:A:161:ARG:NH1	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	175/212 (82%)	146 (83%)	26 (15%)	3 (2%)	14	42
1	B	174/212 (82%)	154 (88%)	16 (9%)	4 (2%)	10	31
1	C	174/212 (82%)	161 (92%)	11 (6%)	2 (1%)	21	57
1	D	174/212 (82%)	157 (90%)	15 (9%)	2 (1%)	21	57
All	All	697/848 (82%)	618 (89%)	68 (10%)	11 (2%)	14	44

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ILE
1	A	169	ASP
1	C	150	GLY
1	A	150	GLY
1	B	150	GLY
1	B	169	ASP
1	B	82	ILE
1	D	150	GLY
1	C	191	VAL
1	D	168	ALA
1	B	191	VAL

### 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	140/168 (83%)	123 (88%)	17 (12%)	7	21
1	B	139/168 (83%)	129 (93%)	10 (7%)	21	50
1	C	139/168 (83%)	126 (91%)	13 (9%)	13	34
1	D	139/168 (83%)	126 (91%)	13 (9%)	13	34
All	All	557/672 (83%)	504 (90%)	53 (10%)	12	33

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	5	LEU
1	A	7	ARG
1	A	11	ASN
1	A	30	ILE
1	A	49	SER
1	A	55	SER
1	A	72	GLU
1	A	82	ILE
1	A	83	SER
1	A	98	ASN
1	A	126	ASN

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Mol	Chain	Res	Type
1	A	131	ILE
1	A	136	GLU
1	A	151	LYS
1	A	172	GLN
1	A	176	ILE
1	B	1	MET
1	B	4	ASP
1	B	5	LEU
1	B	98	ASN
1	B	108	VAL
1	B	131	ILE
1	B	136	GLU
1	B	172	GLN
1	B	184	GLN
1	B	191	VAL
1	C	1	MET
1	C	6	ILE
1	C	16	THR
1	C	21	LEU
1	C	22	LYS
1	C	28	HIS
1	C	98	ASN
1	C	108	VAL
1	C	121	SER
1	C	128	ILE
1	C	179	ILE
1	C	187	GLU
1	C	188	LYS
1	D	5	LEU
1	D	17	LEU
1	D	22	LYS
1	D	55	SER
1	D	72	GLU
1	D	82	ILE
1	D	83	SER
1	D	108	VAL
1	D	128	ILE
1	D	172	GLN
1	D	175	HIS
1	D	176	ILE
1	D	192	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such



sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	11	ASN
1	A	26	ASN
1	A	98	ASN
1	A	172	GLN
1	B	8	ASN
1	B	26	ASN
1	B	28	HIS
1	B	98	ASN
1	B	164	HIS
1	C	3	GLN
1	C	8	ASN
1	C	11	ASN
1	C	26	ASN
1	C	98	ASN
1	D	11	ASN
1	D	28	HIS
1	D	98	ASN
1	D	172	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

1 ligand is 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	I22	B	900	-	17,17,17	3.35	9 (52%)	24,24,24	3.04	10 (41%)

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	I22	B	900	-	-	1/24/24/24	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	900	I22	P1-O7	8.25	1.88	1.60
2	B	900	I22	O1-C1	4.74	1.57	1.41
2	B	900	I22	O5-C5	4.72	1.54	1.43
2	B	900	I22	C7-C6	4.47	1.58	1.51
2	B	900	I22	O3-C3	3.97	1.50	1.42
2	B	900	I22	O6-C6	3.07	1.50	1.43
2	B	900	I22	C4-C5	2.76	1.59	1.53
2	B	900	I22	P1-O10	2.70	1.64	1.54
2	B	900	I22	O7-C7	2.49	1.55	1.44

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	900	I22	C6-C5-C4	-5.80	102.99	112.43
2	B	900	I22	O4-C4-C5	-5.61	95.88	109.42
2	B	900	I22	O3-C3-C2	5.22	119.67	111.16
2	B	900	I22	O5-C5-C6	-5.12	95.80	108.74
2	B	900	I22	C5-C4-C3	-4.59	105.47	113.71
2	B	900	I22	O6-C6-C7	-4.36	101.17	110.12
2	B	900	I22	O3-C3-C4	-4.35	101.28	110.49
2	B	900	I22	O6-C6-C5	3.66	118.16	109.05
2	B	900	I22	C1-C2-C3	3.62	123.11	116.26
2	B	900	I22	O5-C5-C4	-2.65	103.02	109.42

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	900	I22	O2-C2-C1-O1

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	179/212 (84%)	-0.47	1 (0%) 86 88	27, 43, 68, 84	0
1	B	178/212 (83%)	-0.51	0 100 100	22, 41, 68, 79	0
1	C	178/212 (83%)	-0.47	1 (0%) 86 88	22, 41, 67, 82	0
1	D	178/212 (83%)	-0.47	0 100 100	22, 43, 69, 84	0
All	All	713/848 (84%)	-0.48	2 (0%) 91 93	22, 42, 68, 84	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	166	GLY	3.7
1	A	191	VAL	3.1

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

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

### 6.3 Carbohydrates

There are no carbohydrates in this entry.

### 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	I22	B	900	18/18	0.33	5.17	22,28,32,36	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.