



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:39 AM GMT

PDB ID : 2HZM  
Title : Structure of the Mediator head subcomplex Med18/20  
Authors : Lariviere, L.; Geiger, S.; Hoepfner, S.; Rother, S.; Straesser, K.; Cramer, P.  
Deposited on : 2006-08-09  
Resolution : 2.40 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

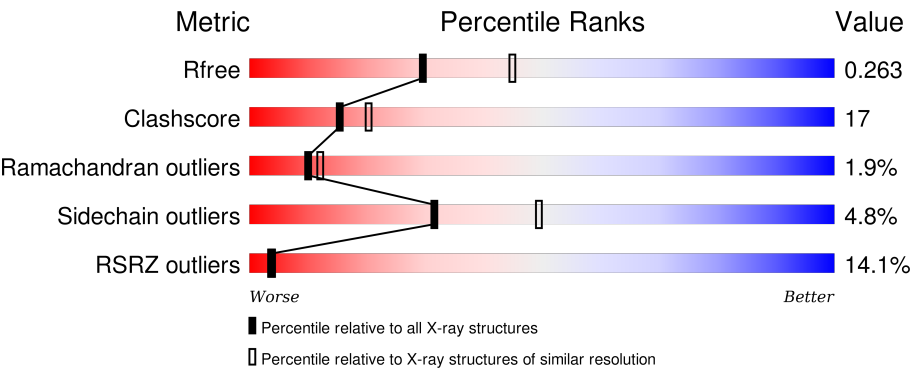
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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 <sub>free</sub>	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	212	<div><div>3%</div><div>74%</div><div>19%</div><div>• •</div></div>
1	C	212	<div><div>9%</div><div>65%</div><div>23%</div><div>• 8%</div></div>
1	E	212	<div><div>26%</div><div>55%</div><div>34%</div><div>• 7%</div></div>
1	G	212	<div><div>31%</div><div>56%</div><div>34%</div><div>• 8%</div></div>
2	B	317	<div><div>5%</div><div>50%</div><div>18%</div><div>• • 28%</div></div>

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Mol	Chain	Length	Quality of chain
2	D	317	<div><div><div></div><div></div><div></div><div></div></div><div>7%51%19%•26%</div></div>
2	F	317	<div><div><div></div><div></div><div></div><div></div></div><div>4%56%17%•25%</div></div>
2	H	317	<div><div><div></div><div></div><div></div><div></div></div><div>15%45%24%••29%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13587 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 RNA polymerase II mediator complex subunit 20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1574	994	265	310	5			
1	C	195	Total	C	N	O	S	0	0	0
			1504	952	253	294	5			
1	E	197	Total	C	N	O	S	0	0	0
			1520	961	257	297	5			
1	G	196	Total	C	N	O	S	0	0	0
			1511	957	254	295	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	CLONING ARTIFACT	UNP P34162
A	0	SER	-	CLONING ARTIFACT	UNP P34162
C	-1	ALA	-	CLONING ARTIFACT	UNP P34162
C	0	SER	-	CLONING ARTIFACT	UNP P34162
E	-1	ALA	-	CLONING ARTIFACT	UNP P34162
E	0	SER	-	CLONING ARTIFACT	UNP P34162
G	-1	ALA	-	CLONING ARTIFACT	UNP P34162
G	0	SER	-	CLONING ARTIFACT	UNP P34162

- Molecule 2 is a protein called RNA polymerase II mediator complex subunit 18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1785	1145	291	342	7			
2	D	233	Total	C	N	O	S	0	0	0
			1820	1165	299	347	9			
2	F	238	Total	C	N	O	S	0	0	0
			1869	1199	302	358	10			
2	H	226	Total	C	N	O	S	0	0	0
			1770	1137	287	337	9			

There are 48 discrepancies between the modelled and reference sequences:

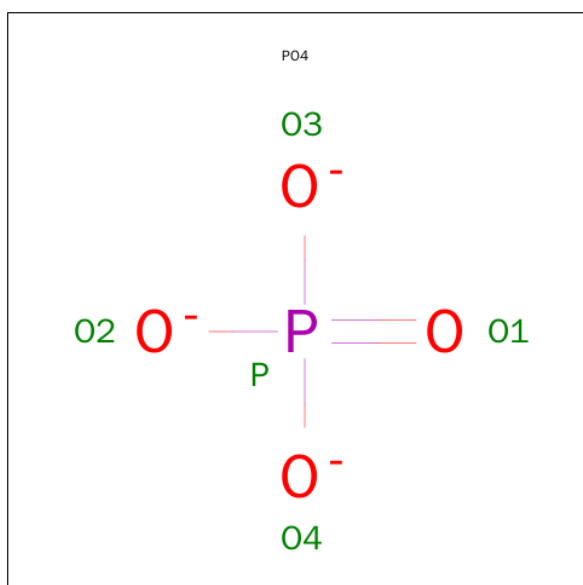
Chain	Residue	Modelled	Actual	Comment	Reference
B	274	VAL	ALA	ENGINEERED	UNP P32585
B	308	ALA	-	CLONING ARTIFACT	UNP P32585
B	309	ALA	-	CLONING ARTIFACT	UNP P32585
B	310	ALA	-	CLONING ARTIFACT	UNP P32585
B	311	LEU	-	CLONING ARTIFACT	UNP P32585
B	312	GLU	-	CLONING ARTIFACT	UNP P32585
B	313	HIS	-	EXPRESSION TAG	UNP P32585
B	314	HIS	-	EXPRESSION TAG	UNP P32585
B	315	HIS	-	EXPRESSION TAG	UNP P32585
B	316	HIS	-	EXPRESSION TAG	UNP P32585
B	317	HIS	-	EXPRESSION TAG	UNP P32585
B	318	HIS	-	EXPRESSION TAG	UNP P32585
D	274	VAL	ALA	ENGINEERED	UNP P32585
D	308	ALA	-	CLONING ARTIFACT	UNP P32585
D	309	ALA	-	CLONING ARTIFACT	UNP P32585
D	310	ALA	-	CLONING ARTIFACT	UNP P32585
D	311	LEU	-	CLONING ARTIFACT	UNP P32585
D	312	GLU	-	CLONING ARTIFACT	UNP P32585
D	313	HIS	-	EXPRESSION TAG	UNP P32585
D	314	HIS	-	EXPRESSION TAG	UNP P32585
D	315	HIS	-	EXPRESSION TAG	UNP P32585
D	316	HIS	-	EXPRESSION TAG	UNP P32585
D	317	HIS	-	EXPRESSION TAG	UNP P32585
D	318	HIS	-	EXPRESSION TAG	UNP P32585
F	274	VAL	ALA	ENGINEERED	UNP P32585
F	308	ALA	-	CLONING ARTIFACT	UNP P32585
F	309	ALA	-	CLONING ARTIFACT	UNP P32585
F	310	ALA	-	CLONING ARTIFACT	UNP P32585
F	311	LEU	-	CLONING ARTIFACT	UNP P32585
F	312	GLU	-	CLONING ARTIFACT	UNP P32585
F	313	HIS	-	EXPRESSION TAG	UNP P32585
F	314	HIS	-	EXPRESSION TAG	UNP P32585
F	315	HIS	-	EXPRESSION TAG	UNP P32585
F	316	HIS	-	EXPRESSION TAG	UNP P32585
F	317	HIS	-	EXPRESSION TAG	UNP P32585
F	318	HIS	-	EXPRESSION TAG	UNP P32585
H	274	VAL	ALA	ENGINEERED	UNP P32585
H	308	ALA	-	CLONING ARTIFACT	UNP P32585
H	309	ALA	-	CLONING ARTIFACT	UNP P32585
H	310	ALA	-	CLONING ARTIFACT	UNP P32585
H	311	LEU	-	CLONING ARTIFACT	UNP P32585
H	312	GLU	-	CLONING ARTIFACT	UNP P32585

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Chain	Residue	Modelled	Actual	Comment	Reference
H	313	HIS	-	EXPRESSION TAG	UNP P32585
H	314	HIS	-	EXPRESSION TAG	UNP P32585
H	315	HIS	-	EXPRESSION TAG	UNP P32585
H	316	HIS	-	EXPRESSION TAG	UNP P32585
H	317	HIS	-	EXPRESSION TAG	UNP P32585
H	318	HIS	-	EXPRESSION TAG	UNP P32585

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	76	Total O 76 76	0	0
4	B	40	Total O 40 40	0	0
4	C	16	Total O 16 16	0	0
4	D	41	Total O 41 41	0	0
4	E	6	Total O 6 6	0	0

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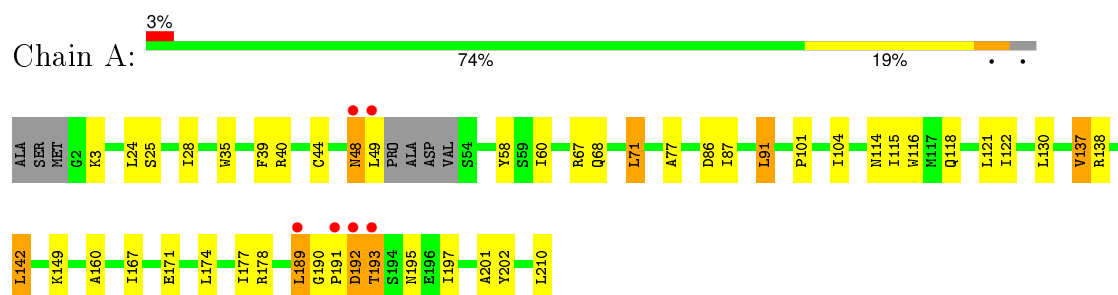
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	40	Total 40	O 40	0	0
4	G	2	Total 2	O 2	0	0
4	H	8	Total 8	O 8	0	0

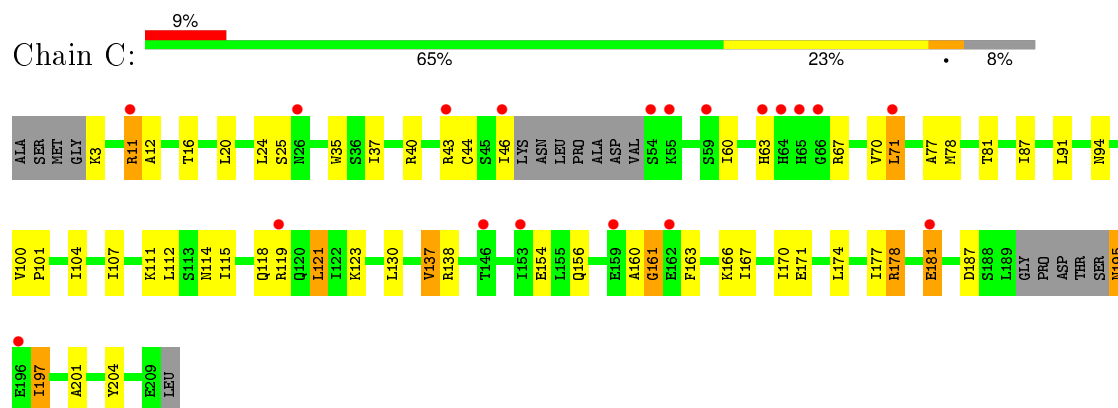
### 3 Residue-property plots

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

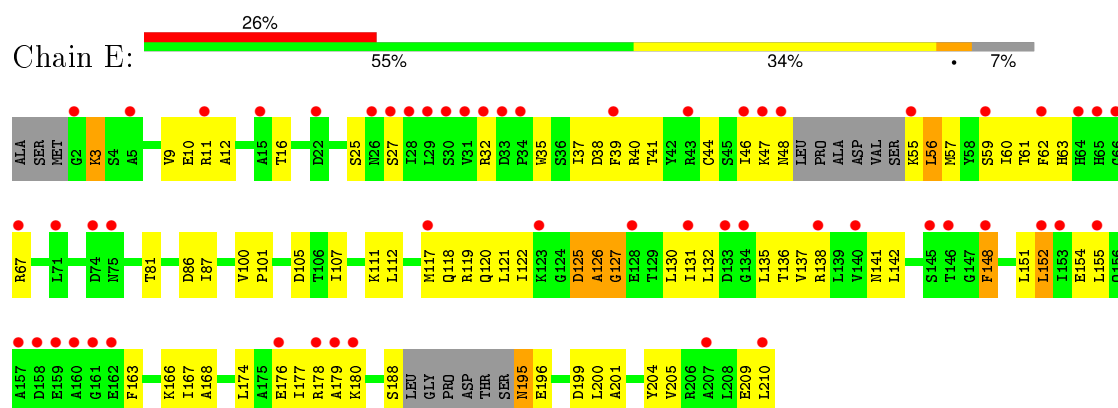
- Molecule 1: RNA polymerase II mediator complex subunit 20



- Molecule 1: RNA polymerase II mediator complex subunit 20

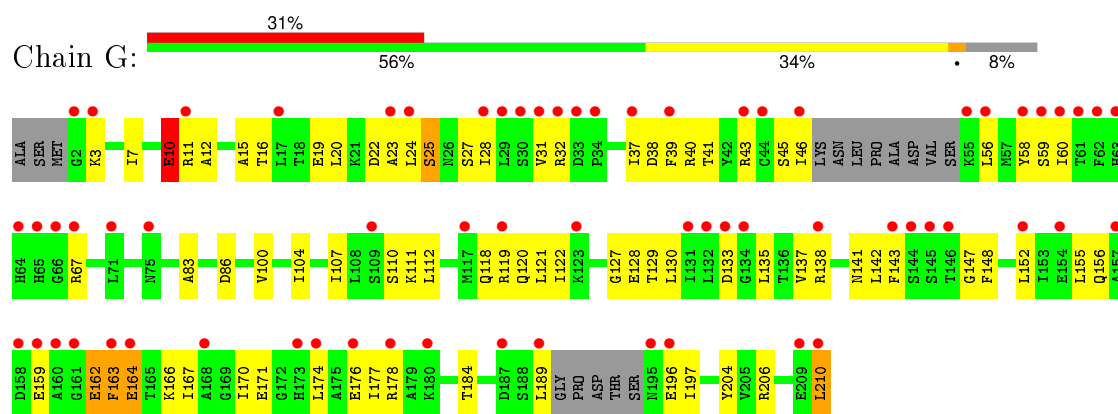


- Molecule 1: RNA polymerase II mediator complex subunit 20

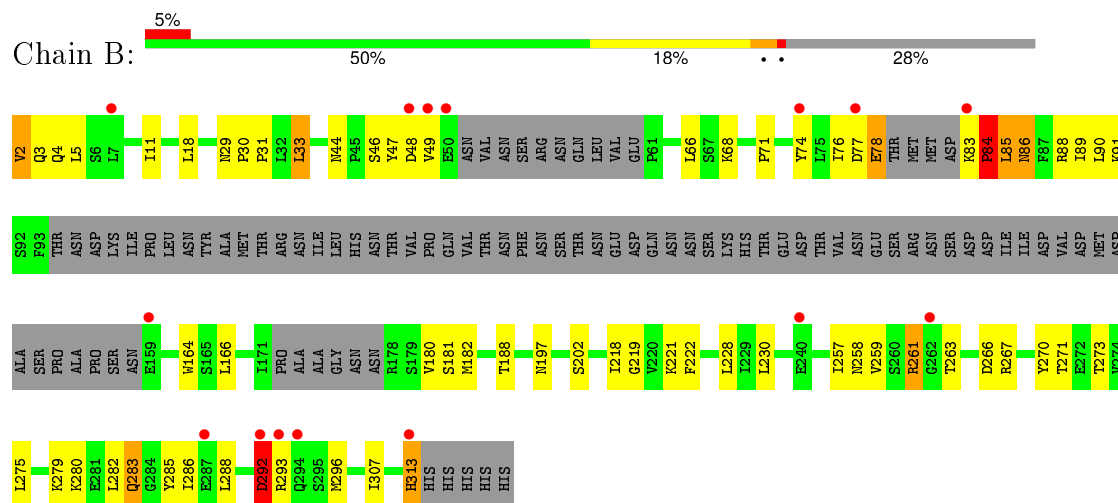


- Molecule 1: RNA polymerase II mediator complex subunit 20

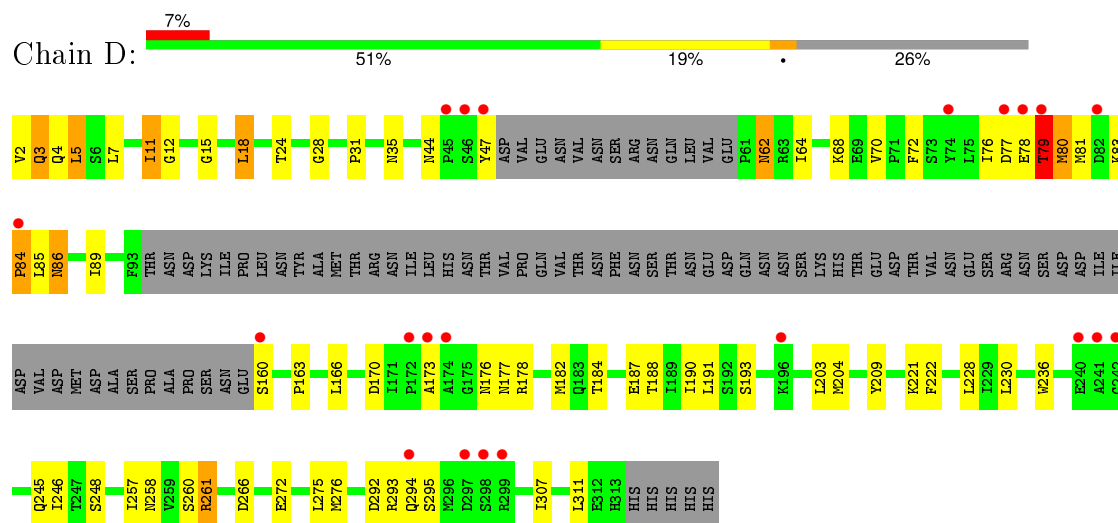




- Molecule 2: RNA polymerase II mediator complex subunit 18

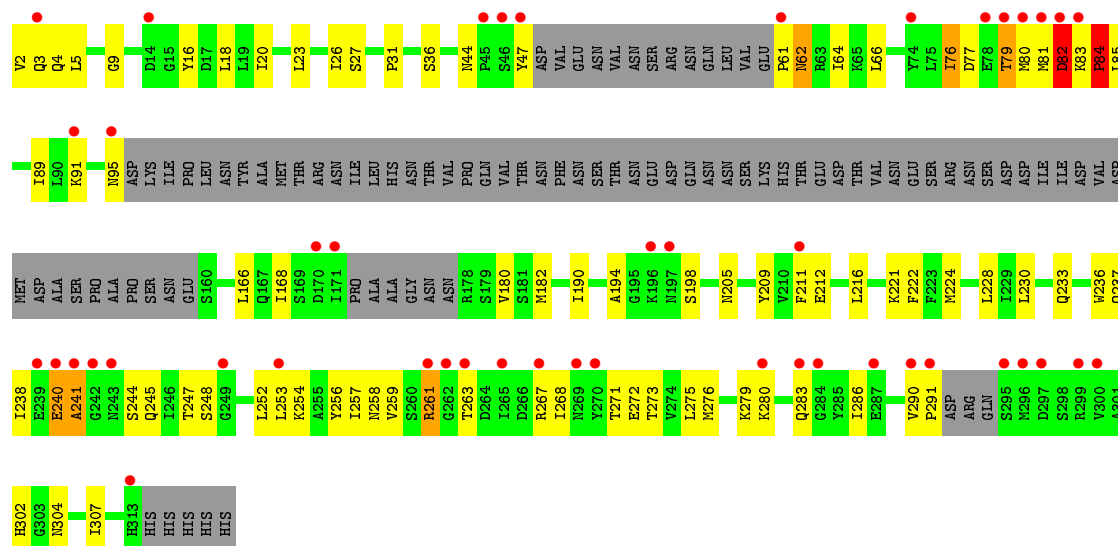


- Molecule 2: RNA polymerase II mediator complex subunit 18



- Molecule 2: RNA polymerase II mediator complex subunit 18





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.90Å 129.35Å 241.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40 19.98 – 2.40	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.40) 98.7 (19.98-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.24 (at 2.41Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.228 , 0.264 0.228 , 0.263	Depositor DCC
$R_{free}$ test set	4276 reflections (4.81%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.8	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 56.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 88929 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13587	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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	0.52	0/1598	0.72	0/2162
1	C	0.36	0/1526	0.60	0/2064
1	E	0.31	0/1542	0.54	0/2083
1	G	0.34	0/1533	0.58	0/2072
2	B	0.48	0/1816	0.75	3/2453 (0.1%)
2	D	0.43	0/1854	0.68	1/2508 (0.0%)
2	F	0.44	0/1903	0.67	0/2573
2	H	0.36	0/1801	0.63	2/2433 (0.1%)
All	All	0.42	0/13573	0.65	6/18348 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	84	PRO	N-CA-C	7.68	132.08	112.10
2	H	82	ASP	N-CA-C	6.66	128.98	111.00
2	H	241	ALA	N-CA-C	-6.21	94.22	111.00
2	B	85	LEU	CA-CB-CG	5.80	128.65	115.30
2	D	79	THR	N-CA-C	-5.28	96.73	111.00
2	B	33	LEU	CA-CB-CG	5.28	127.43	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1574	0	1588	36	0
1	C	1504	0	1517	45	0
1	E	1520	0	1534	77	0
1	G	1511	0	1526	81	0
2	B	1785	0	1799	68	0
2	D	1820	0	1837	68	0
2	F	1869	0	1885	42	0
2	H	1770	0	1791	74	0
3	A	5	0	0	0	0
4	A	76	0	0	0	0
4	B	40	0	0	1	0
4	C	16	0	0	0	0
4	D	41	0	0	0	0
4	E	6	0	0	0	0
4	F	40	0	0	1	0
4	G	2	0	0	0	0
4	H	8	0	0	0	0
All	All	13587	0	13477	465	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 17.

All (465) 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)
2:B:83:LYS:HB3	2:B:84:PRO:HD2	1.20	1.07
1:A:114:ASN:HD22	2:B:49:VAL:HG11	1.24	1.02
1:E:40:ARG:HH11	1:E:118:GLN:HE22	1.10	0.95
2:B:83:LYS:CB	2:B:84:PRO:HD2	1.96	0.95
2:B:4:GLN:HE21	2:B:258:ASN:HD21	1.16	0.93
2:B:261:ARG:HD3	2:B:261:ARG:H	1.33	0.91
2:D:77:ASP:OD1	2:D:79:THR:HG22	1.71	0.91
1:G:39:PHE:HZ	1:G:204:TYR:HB3	1.35	0.89
2:D:86:ASN:O	2:D:89:ILE:HG13	1.74	0.88
1:E:142:LEU:HD11	1:E:152:LEU:HD12	1.55	0.87
1:E:41:THR:HB	1:E:120:GLN:HB2	1.57	0.87
2:H:83:LYS:HE2	2:H:83:LYS:HA	1.56	0.86
1:C:40:ARG:HH11	1:C:118:GLN:HE22	1.23	0.85
1:G:31:VAL:HG12	1:G:32:ARG:H	1.42	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:263:THR:CG2	2:F:267:ARG:HD3	2.09	0.83
2:D:178:ARG:HG3	2:D:182:MET:HE3	1.60	0.82
1:C:163:PHE:O	1:C:167:ILE:HD12	1.81	0.81
1:E:44:CYS:HB3	1:E:55:LYS:HB3	1.63	0.81
1:E:135:LEU:HD12	1:E:166:LYS:HB3	1.61	0.81
1:A:49:LEU:HG	2:B:47:TYR:HE1	1.47	0.80
2:D:44:ASN:HB3	2:D:47:TYR:CD2	2.18	0.79
2:F:5:LEU:CD2	2:F:182:MET:HG3	2.13	0.79
1:G:20:LEU:O	1:G:24:LEU:HD13	1.83	0.78
2:D:261:ARG:CD	2:D:261:ARG:H	1.95	0.78
2:B:83:LYS:HB3	2:B:84:PRO:CD	2.09	0.76
2:F:86:ASN:O	2:F:89:ILE:HG12	1.84	0.76
2:D:4:GLN:HE21	2:D:258:ASN:HD21	1.34	0.76
2:D:173:ALA:HA	2:D:176:ASN:ND2	2.01	0.75
1:G:130:LEU:HB2	1:G:137:VAL:HG23	1.69	0.75
2:F:261:ARG:HE	2:F:261:ARG:H	1.31	0.74
2:H:238:ILE:HG23	2:H:240:GLU:OE2	1.86	0.74
1:A:48:ASN:O	1:A:49:LEU:HB2	1.86	0.74
2:D:261:ARG:H	2:D:261:ARG:HD3	1.50	0.74
2:D:85:LEU:HD12	2:D:89:ILE:HD13	1.68	0.74
2:D:11:ILE:HD13	2:D:12:GLY:H	1.53	0.74
1:C:100:VAL:HB	2:D:2:VAL:HG21	1.70	0.73
1:E:135:LEU:HD23	1:E:136:THR:N	2.03	0.73
2:D:76:ILE:HG13	2:D:80:MET:HG2	1.69	0.73
2:H:280:LYS:O	2:H:283:GLN:HG2	1.88	0.73
1:C:20:LEU:O	1:C:24:LEU:HD13	1.89	0.73
2:D:11:ILE:HD13	2:D:12:GLY:N	2.03	0.72
2:D:5:LEU:HD22	2:D:182:MET:HG3	1.71	0.72
2:D:178:ARG:HD2	2:D:272:GLU:OE1	1.89	0.71
2:D:261:ARG:N	2:D:261:ARG:HD3	2.04	0.71
1:E:100:VAL:HG11	2:F:261:ARG:HH22	1.55	0.71
2:D:76:ILE:HG23	2:D:80:MET:HB3	1.72	0.71
2:H:240:GLU:HA	2:H:240:GLU:OE1	1.89	0.70
2:B:85:LEU:HD12	2:B:89:ILE:HD13	1.73	0.70
2:H:44:ASN:HB3	2:H:47:TYR:CD2	2.26	0.70
1:C:130:LEU:HB2	1:C:137:VAL:HG13	1.73	0.69
2:D:44:ASN:HB3	2:D:47:TYR:HD2	1.56	0.69
2:H:4:GLN:HE21	2:H:258:ASN:HD21	1.39	0.69
1:G:39:PHE:CZ	1:G:204:TYR:HB3	2.25	0.69
1:G:60:ILE:HD12	1:G:60:ILE:N	2.08	0.68
2:H:4:GLN:HG3	2:H:258:ASN:ND2	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:160:SER:N	2:D:193:SER:HG	1.90	0.68
1:A:49:LEU:HG	2:B:47:TYR:CE1	2.29	0.68
1:A:114:ASN:HD22	2:B:49:VAL:CG1	2.04	0.68
1:G:135:LEU:HD12	1:G:166:LYS:HE2	1.76	0.68
1:E:119:ARG:O	1:E:120:GLN:HG2	1.94	0.67
2:F:85:LEU:HD23	2:F:88:ARG:HE	1.60	0.67
2:B:85:LEU:HA	2:B:89:ILE:HD11	1.76	0.67
2:F:263:THR:HG21	2:F:267:ARG:HD3	1.76	0.67
1:C:40:ARG:HH11	1:C:118:GLN:NE2	1.91	0.67
2:B:261:ARG:N	2:B:261:ARG:HD3	2.08	0.66
1:G:25:SER:HA	1:G:28:ILE:HG13	1.75	0.66
1:G:120:GLN:HE21	1:G:122:ILE:HG13	1.60	0.66
1:A:167:ILE:O	1:A:171:GLU:HG3	1.94	0.66
2:B:85:LEU:HD12	2:B:89:ILE:CD1	2.26	0.66
2:D:78:GLU:HA	2:D:81:MET:HG2	1.77	0.65
2:H:4:GLN:HG3	2:H:258:ASN:HD21	1.62	0.65
1:G:60:ILE:HD12	1:G:60:ILE:H	1.62	0.65
1:G:25:SER:HA	1:G:28:ILE:CD1	2.26	0.65
1:E:67:ARG:HD2	1:E:67:ARG:N	2.12	0.65
2:H:263:THR:HB	2:H:267:ARG:HD2	1.79	0.65
1:G:137:VAL:HG12	1:G:155:LEU:CD2	2.27	0.64
1:G:31:VAL:HG12	1:G:32:ARG:N	2.10	0.64
1:E:60:ILE:HD12	1:E:60:ILE:N	2.13	0.64
1:G:20:LEU:HD13	1:G:177:ILE:HD13	1.80	0.64
1:C:170:ILE:O	1:C:174:LEU:HD13	1.98	0.64
1:G:137:VAL:HG12	1:G:155:LEU:HD22	1.80	0.64
2:D:7:LEU:HD11	2:D:276:MET:CE	2.28	0.64
1:E:56:LEU:N	1:E:56:LEU:HD23	2.12	0.63
2:B:270:TYR:O	2:B:273:THR:HB	1.99	0.63
2:H:77:ASP:OD1	2:H:79:THR:HG23	1.98	0.63
2:F:91:LYS:HD3	4:F:348:HOH:O	1.97	0.63
1:A:193:THR:HG22	1:A:193:THR:O	1.98	0.63
1:G:23:ALA:C	1:G:24:LEU:HD12	2.19	0.63
1:A:40:ARG:HE	1:A:118:GLN:HE22	1.46	0.62
1:G:25:SER:HA	1:G:28:ILE:CG1	2.29	0.62
2:H:85:LEU:HG	2:H:89:ILE:HD11	1.80	0.62
2:B:166:LEU:HD23	2:B:166:LEU:C	2.19	0.62
1:C:114:ASN:ND2	1:C:115:ILE:HG13	2.14	0.62
1:E:87:ILE:HG12	2:F:189:ILE:HG13	1.80	0.62
2:D:261:ARG:CD	2:D:261:ARG:N	2.62	0.61
1:G:206:ARG:HH11	1:G:206:ARG:HG3	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ILE:HD13	1:C:201:ALA:HB1	1.81	0.61
1:A:130:LEU:HB2	1:A:137:VAL:HG22	1.83	0.61
1:E:195:ASN:HD22	1:E:196:GLU:N	1.98	0.61
2:H:80:MET:SD	2:H:91:LYS:HD3	2.41	0.61
2:F:5:LEU:HD22	2:F:182:MET:HG3	1.82	0.61
2:B:71:PRO:HG2	2:B:74:TYR:CD1	2.36	0.61
2:H:253:LEU:HD23	2:H:286:ILE:HD13	1.84	0.60
1:G:58:TYR:HE2	1:G:210:LEU:HD22	1.65	0.60
1:E:11:ARG:HB2	1:E:180:LYS:HB2	1.83	0.60
1:A:60:ILE:HD13	1:A:201:ALA:HB1	1.84	0.60
1:G:119:ARG:HG3	1:G:119:ARG:HH11	1.66	0.60
2:H:23:LEU:O	2:H:27:SER:HB3	2.01	0.59
1:E:126:ALA:O	1:E:127:GLY:C	2.41	0.59
1:G:100:VAL:HB	2:H:2:VAL:CG2	2.32	0.59
2:B:261:ARG:CD	2:B:261:ARG:H	2.02	0.59
1:E:135:LEU:CD1	1:E:166:LYS:HB3	2.30	0.59
1:G:100:VAL:HB	2:H:2:VAL:HG21	1.83	0.59
1:G:138:ARG:NH2	1:G:156:GLN:HE21	1.99	0.59
1:G:142:LEU:HD21	1:G:152:LEU:HD12	1.83	0.59
2:F:102:TYR:O	2:F:103:ALA:CB	2.51	0.59
1:E:174:LEU:HD12	1:E:177:ILE:HD11	1.84	0.58
2:D:85:LEU:HA	2:D:89:ILE:HD11	1.85	0.58
1:A:142:LEU:HD13	1:A:149:LYS:HD3	1.86	0.58
1:G:119:ARG:NH1	1:G:119:ARG:HG3	2.19	0.58
1:G:25:SER:HA	1:G:28:ILE:HD12	1.85	0.58
1:E:125:ASP:O	1:E:126:ALA:CB	2.51	0.58
1:G:163:PHE:O	1:G:166:LYS:N	2.37	0.58
1:C:40:ARG:NH1	1:C:118:GLN:HE22	1.97	0.58
2:F:4:GLN:HE21	2:F:258:ASN:HD21	1.52	0.58
2:D:7:LEU:HD11	2:D:276:MET:HE1	1.84	0.57
1:E:3:LYS:HG3	1:E:196:GLU:OE2	2.03	0.57
1:C:63:HIS:CE1	1:C:67:ARG:HE	2.22	0.57
1:G:43:ARG:HA	1:G:56:LEU:HD23	1.86	0.57
2:H:64:ILE:HG12	2:H:168:ILE:HG12	1.85	0.57
2:H:23:LEU:HD22	2:H:230:LEU:HD23	1.87	0.57
1:G:40:ARG:NE	1:G:118:GLN:NE2	2.51	0.57
2:B:85:LEU:CA	2:B:89:ILE:HD11	2.35	0.57
2:D:64:ILE:HG21	2:D:204:MET:HE1	1.86	0.57
1:A:35:TRP:CZ2	1:A:138:ARG:HB3	2.40	0.56
2:B:90:LEU:HD11	2:B:219:GLY:HA2	1.87	0.56
2:H:259:VAL:CG2	2:H:267:ARG:HD3	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:ASN:HD22	2:D:35:ASN:H	1.53	0.56
2:D:3:GLN:NE2	2:D:184:THR:OG1	2.36	0.56
2:D:292:ASP:OD2	2:D:295:SER:HB2	2.05	0.56
2:H:5:LEU:HD12	2:H:271:THR:CG2	2.35	0.56
1:C:167:ILE:H	1:C:167:ILE:HD12	1.71	0.56
2:B:86:ASN:N	2:B:89:ILE:HD11	2.21	0.56
2:F:221:LYS:HA	2:F:230:LEU:O	2.05	0.56
1:G:100:VAL:CG1	2:H:261:ARG:HH12	2.19	0.56
2:H:257:ILE:HG13	2:H:275:LEU:HD11	1.86	0.56
1:C:44:CYS:SG	1:C:46:ILE:HD13	2.45	0.56
1:A:114:ASN:ND2	1:A:115:ILE:HG13	2.21	0.56
2:D:85:LEU:HD12	2:D:89:ILE:CD1	2.36	0.56
1:C:87:ILE:HD11	1:C:101:PRO:HG3	1.87	0.56
2:B:86:ASN:HD22	2:B:86:ASN:C	2.09	0.55
1:G:130:LEU:HB2	1:G:137:VAL:CG2	2.35	0.55
1:E:44:CYS:SG	1:E:46:ILE:HD13	2.46	0.55
1:C:195:ASN:HD22	1:C:195:ASN:C	2.09	0.55
1:G:163:PHE:O	1:G:164:GLU:C	2.45	0.55
1:A:39:PHE:HB2	1:A:122:ILE:CG1	2.36	0.55
2:H:180:VAL:HG22	2:H:272:GLU:HG3	1.87	0.55
2:D:163:PRO:HA	2:D:190:ILE:O	2.07	0.55
2:F:102:TYR:O	2:F:103:ALA:HB3	2.06	0.55
2:B:263:THR:HG22	2:B:267:ARG:HB3	1.89	0.54
1:E:40:ARG:NH1	1:E:118:GLN:HE22	1.93	0.54
2:B:33:LEU:HD21	2:B:89:ILE:HD12	1.90	0.54
2:H:61:PRO:HG2	2:H:62:ASN:H	1.70	0.54
2:F:77:ASP:OD1	2:F:80:MET:HG3	2.07	0.54
1:C:160:ALA:O	1:C:161:GLY:O	2.25	0.54
1:A:77:ALA:HB2	1:A:189:LEU:HD21	1.88	0.54
2:H:76:ILE:HD11	2:H:89:ILE:HA	1.90	0.54
2:D:293:ARG:C	2:D:295:SER:H	2.11	0.54
2:D:5:LEU:CD2	2:D:182:MET:HG3	2.38	0.54
2:H:5:LEU:HD21	2:H:182:MET:CE	2.38	0.54
2:D:44:ASN:HB3	2:D:47:TYR:CE2	2.43	0.53
1:E:67:ARG:H	1:E:67:ARG:HD2	1.73	0.53
1:A:40:ARG:HE	1:A:118:GLN:NE2	2.06	0.53
2:B:5:LEU:HD21	2:B:182:MET:CE	2.38	0.53
1:E:48:ASN:N	1:E:55:LYS:NZ	2.57	0.53
1:G:40:ARG:HE	1:G:118:GLN:NE2	2.07	0.53
2:D:31:PRO:HB3	2:D:222:PHE:CZ	2.44	0.53
1:C:37:ILE:HD13	1:C:204:TYR:CE1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:58:TYR:CE2	1:G:210:LEU:HD22	2.42	0.53
1:G:141:ASN:HB3	1:G:143:PHE:HE1	1.73	0.53
2:H:83:LYS:CE	2:H:83:LYS:HA	2.27	0.53
2:H:254:LYS:HE2	2:H:256:TYR:CD2	2.44	0.53
2:B:86:ASN:HD21	2:B:88:ARG:HB2	1.72	0.53
2:F:252:LEU:HD22	2:F:310:ALA:HB2	1.91	0.53
2:B:44:ASN:HB3	2:B:47:TYR:CD2	2.44	0.53
1:E:122:ILE:O	1:E:122:ILE:HG13	2.08	0.53
1:G:22:ASP:C	1:G:24:LEU:H	2.12	0.52
1:E:188:SER:HA	1:E:199:ASP:OD1	2.09	0.52
1:C:78:MET:HB2	2:D:203:LEU:HD22	1.90	0.52
1:E:163:PHE:O	1:E:166:LYS:HB2	2.09	0.52
2:D:173:ALA:HA	2:D:176:ASN:HD21	1.73	0.52
2:D:86:ASN:HD22	2:D:86:ASN:C	2.13	0.52
2:H:166:LEU:HD12	2:H:190:ILE:HD11	1.92	0.52
2:D:24:THR:O	2:D:28:GLY:N	2.42	0.52
1:E:100:VAL:HG11	2:F:261:ARG:NH2	2.24	0.52
2:H:36:SER:O	2:H:216:LEU:HD12	2.09	0.52
2:H:85:LEU:O	2:H:89:ILE:HG13	2.10	0.52
2:H:304:ASN:CG	2:H:307:ILE:HD13	2.30	0.51
1:E:25:SER:C	1:E:27:SER:H	2.14	0.51
2:H:82:ASP:O	2:H:83:LYS:HG2	2.10	0.51
2:B:5:LEU:CD2	2:B:182:MET:HG3	2.40	0.51
1:G:31:VAL:O	1:G:32:ARG:HG3	2.10	0.51
2:H:259:VAL:HG21	2:H:267:ARG:HD3	1.91	0.51
1:E:11:ARG:CB	1:E:180:LYS:HB2	2.40	0.51
2:B:68:LYS:HE2	2:B:164:TRP:CZ2	2.46	0.51
2:F:46:SER:C	2:F:47:TYR:HD1	2.14	0.51
1:E:46:ILE:HG22	1:E:47:LYS:N	2.26	0.51
2:H:85:LEU:HG	2:H:89:ILE:CD1	2.39	0.51
1:G:3:LYS:HG3	1:G:196:GLU:OE2	2.09	0.51
1:E:10:GLU:N	1:E:10:GLU:OE2	2.34	0.51
1:E:130:LEU:HB2	1:E:137:VAL:CG2	2.41	0.51
2:D:246:ILE:HG23	2:D:311:LEU:HD23	1.93	0.51
2:H:5:LEU:HD21	2:H:182:MET:HE2	1.93	0.51
2:D:86:ASN:N	2:D:89:ILE:HD11	2.26	0.50
2:D:64:ILE:HG21	2:D:204:MET:CE	2.41	0.50
1:E:46:ILE:HG22	1:E:55:LYS:NZ	2.27	0.50
2:F:239:GLU:HB2	2:F:242:GLY:O	2.11	0.50
1:G:111:LYS:C	1:G:112:LEU:HD12	2.31	0.50
1:G:67:ARG:HH11	1:G:67:ARG:HG3	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:ARG:HB2	1:E:154:GLU:HB3	1.94	0.50
2:B:221:LYS:HA	2:B:230:LEU:O	2.11	0.50
1:E:56:LEU:H	1:E:56:LEU:HD23	1.75	0.50
2:H:80:MET:CE	2:H:91:LYS:HD3	2.41	0.50
1:C:63:HIS:CE1	1:C:67:ARG:NE	2.79	0.50
2:H:83:LYS:O	2:H:84:PRO:C	2.50	0.50
2:B:29:ASN:HB3	2:B:30:PRO:HD2	1.93	0.50
1:G:171:GLU:HA	1:G:174:LEU:HB2	1.94	0.50
1:A:25:SER:HA	1:A:28:ILE:HG13	1.94	0.50
2:H:18:LEU:C	2:H:18:LEU:HD13	2.32	0.50
1:E:137:VAL:HG12	1:E:155:LEU:CD2	2.42	0.50
1:A:87:ILE:HD11	1:A:101:PRO:HG3	1.93	0.50
1:E:46:ILE:CG2	1:E:47:LYS:N	2.74	0.49
1:C:167:ILE:O	1:C:171:GLU:HG3	2.12	0.49
1:C:71:LEU:O	1:C:77:ALA:HA	2.12	0.49
1:E:12:ALA:HB1	1:E:16:THR:OG1	2.13	0.49
2:H:9:GLY:O	2:H:252:LEU:HD12	2.11	0.49
2:B:5:LEU:HA	2:B:181:SER:O	2.13	0.49
2:D:221:LYS:HA	2:D:230:LEU:O	2.13	0.49
1:C:43:ARG:HD2	1:C:119:ARG:HD2	1.94	0.49
1:E:135:LEU:HD12	1:E:166:LYS:HD2	1.93	0.49
2:D:261:ARG:NE	2:D:261:ARG:H	2.11	0.49
1:G:40:ARG:CD	1:G:118:GLN:HE21	2.25	0.49
2:F:300:VAL:HG23	2:F:311:LEU:HD13	1.93	0.49
2:F:228:LEU:HA	2:F:257:ILE:HG12	1.95	0.49
1:E:46:ILE:N	1:E:46:ILE:HD12	2.27	0.49
1:C:11:ARG:HG3	1:C:181:GLU:CB	2.42	0.49
2:H:290:VAL:HG23	2:H:291:PRO:HD2	1.95	0.49
2:H:221:LYS:HA	2:H:230:LEU:O	2.13	0.48
1:G:127:GLY:O	1:G:128:GLU:HG3	2.12	0.48
1:E:56:LEU:CD2	1:E:56:LEU:N	2.76	0.48
1:E:87:ILE:HD11	1:E:101:PRO:HD3	1.95	0.48
1:E:39:PHE:HB3	1:E:122:ILE:CG1	2.43	0.48
2:B:68:LYS:HE2	2:B:164:TRP:CH2	2.47	0.48
1:C:12:ALA:HB1	1:C:16:THR:OG1	2.13	0.48
1:A:58:TYR:CE2	1:A:210:LEU:HB3	2.48	0.48
2:B:4:GLN:NE2	2:B:258:ASN:HD21	1.96	0.48
1:G:40:ARG:NE	1:G:118:GLN:HE21	2.12	0.48
2:H:273:THR:O	2:H:276:MET:HB2	2.14	0.48
1:G:31:VAL:HG13	1:G:129:THR:O	2.13	0.48
1:E:176:GLU:O	1:E:178:ARG:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:85:LEU:C	2:D:89:ILE:HD11	2.34	0.48
2:H:240:GLU:CA	2:H:240:GLU:OE1	2.59	0.48
2:H:276:MET:O	2:H:279:LYS:HB3	2.13	0.48
2:H:194:ALA:C	2:H:198:SER:HB3	2.34	0.48
1:C:91:LEU:HD11	2:D:68:LYS:HA	1.96	0.48
2:F:231:GLU:O	2:F:253:LEU:HD12	2.12	0.48
2:H:205:ASN:ND2	2:H:209:TYR:O	2.42	0.48
2:F:96:ASP:HB3	2:F:244:SER:HA	1.96	0.48
2:H:26:ILE:HG22	2:H:224:MET:CE	2.44	0.48
2:B:11:ILE:HG23	2:B:286:ILE:HD12	1.96	0.48
1:E:107:ILE:CD1	2:F:186:ALA:HB1	2.44	0.48
2:B:44:ASN:OD1	2:B:46:SER:HB3	2.13	0.48
1:G:100:VAL:HG12	2:H:261:ARG:HH12	1.78	0.47
1:C:121:LEU:HD22	1:C:123:LYS:HG3	1.96	0.47
2:D:236:TRP:NE1	2:D:245:GLN:HB2	2.29	0.47
1:C:111:LYS:C	1:C:112:LEU:HD12	2.34	0.47
2:B:313:HIS:H	2:B:313:HIS:CD2	2.32	0.47
1:G:137:VAL:O	1:G:137:VAL:HG23	2.15	0.47
1:A:39:PHE:HB2	1:A:122:ILE:HG13	1.97	0.47
1:E:167:ILE:HG13	1:E:168:ALA:N	2.30	0.47
1:E:125:ASP:O	1:E:126:ALA:HB3	2.15	0.47
1:G:129:THR:O	1:G:130:LEU:HD23	2.15	0.47
1:A:68:GLN:NE2	1:A:197:ILE:CD1	2.78	0.47
1:G:40:ARG:HB2	1:G:59:SER:HB3	1.95	0.47
1:G:163:PHE:HA	1:G:166:LYS:HG3	1.97	0.47
1:E:62:PHE:O	1:E:67:ARG:HA	2.14	0.47
2:B:221:LYS:HE2	4:B:351:HOH:O	2.15	0.47
1:G:83:ALA:HB3	1:G:86:ASP:OD2	2.15	0.47
1:G:31:VAL:CG1	1:G:32:ARG:H	2.21	0.46
1:G:110:SER:O	1:G:111:LYS:HD2	2.15	0.46
1:A:68:GLN:NE2	1:A:197:ILE:HD13	2.30	0.46
1:C:154:GLU:OE2	1:C:156:GLN:NE2	2.46	0.46
2:H:211:PHE:CD1	2:H:212:GLU:N	2.83	0.46
2:D:85:LEU:CA	2:D:89:ILE:HD11	2.44	0.46
1:E:48:ASN:HA	1:E:55:LYS:HE3	1.98	0.46
1:E:67:ARG:H	1:E:67:ARG:CD	2.29	0.46
2:H:23:LEU:HD22	2:H:230:LEU:CD2	2.45	0.46
2:B:182:MET:HB2	2:B:182:MET:HE2	1.79	0.46
2:H:307:ILE:HD12	2:H:307:ILE:N	2.31	0.46
1:A:190:GLY:O	1:A:192:ASP:N	2.39	0.46
2:B:5:LEU:HD12	2:B:271:THR:HG22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:TRP:CZ2	1:E:138:ARG:HB3	2.51	0.46
1:A:44:CYS:HB2	1:A:116:TRP:CZ3	2.50	0.46
1:E:9:VAL:HB	1:E:151:LEU:HB3	1.96	0.46
2:D:166:LEU:HD23	2:D:166:LEU:C	2.35	0.46
2:F:88:ARG:HG2	2:F:88:ARG:HH21	1.81	0.46
1:G:167:ILE:O	1:G:170:ILE:N	2.49	0.46
2:D:85:LEU:HA	2:D:89:ILE:CD1	2.44	0.46
1:C:43:ARG:CD	1:C:119:ARG:HD2	2.45	0.46
2:H:236:TRP:NE1	2:H:245:GLN:HG3	2.29	0.46
2:B:83:LYS:HE3	2:F:85:LEU:CD2	2.46	0.46
1:G:41:THR:OG1	1:G:210:LEU:HD21	2.16	0.46
1:C:11:ARG:HG3	1:C:181:GLU:HB2	1.97	0.46
2:H:26:ILE:HG22	2:H:224:MET:HE1	1.98	0.46
1:C:35:TRP:CE2	1:C:138:ARG:HB3	2.51	0.46
2:H:26:ILE:CG2	2:H:224:MET:HE1	2.46	0.46
1:A:104:ILE:HD13	2:B:188:THR:HG21	1.96	0.46
1:C:177:ILE:O	1:C:178:ARG:HB2	2.14	0.46
2:F:312:GLU:O	2:F:313:HIS:HB2	2.16	0.46
1:C:197:ILE:O	1:C:197:ILE:HD13	2.16	0.46
2:B:5:LEU:HD12	2:B:271:THR:CG2	2.46	0.46
2:D:228:LEU:HA	2:D:257:ILE:HG12	1.97	0.46
1:G:45:SER:C	1:G:46:ILE:HD12	2.36	0.46
1:A:68:GLN:HE21	1:A:197:ILE:CD1	2.29	0.45
2:F:288:LEU:O	2:F:289:SER:HB3	2.16	0.45
2:B:266:ASP:OD2	1:C:3:LYS:HE3	2.15	0.45
2:B:31:PRO:HB3	2:B:222:PHE:CZ	2.51	0.45
2:B:86:ASN:H	2:B:89:ILE:HD11	1.80	0.45
2:D:187:GLU:HG2	2:D:188:THR:N	2.31	0.45
2:B:83:LYS:CB	2:B:84:PRO:CD	2.79	0.45
2:D:11:ILE:HD11	2:D:15:GLY:HA3	1.97	0.45
2:H:4:GLN:NE2	2:H:258:ASN:HD21	2.11	0.45
2:B:279:LYS:HA	2:B:288:LEU:HD12	1.98	0.45
1:E:141:ASN:HB3	1:E:148:PHE:HE1	1.82	0.45
1:G:15:ALA:O	1:G:19:GLU:HG3	2.16	0.45
1:G:174:LEU:HD12	1:G:177:ILE:HD11	1.97	0.45
2:B:88:ARG:O	2:B:91:LYS:HG3	2.17	0.45
1:G:60:ILE:N	1:G:60:ILE:CD1	2.79	0.45
1:A:177:ILE:O	1:A:178:ARG:HB2	2.15	0.45
2:H:247:THR:O	2:H:248:SER:C	2.54	0.45
2:H:31:PRO:HB3	2:H:222:PHE:CZ	2.52	0.45
1:A:48:ASN:O	1:A:49:LEU:CB	2.61	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:178:ARG:HG3	2:D:182:MET:CE	2.39	0.45
2:B:86:ASN:H	2:B:89:ILE:CD1	2.29	0.45
2:H:4:GLN:CG	2:H:258:ASN:HD21	2.29	0.45
1:G:40:ARG:HH11	1:G:40:ARG:HG3	1.81	0.45
1:A:71:LEU:O	1:A:77:ALA:HA	2.17	0.45
2:B:5:LEU:HD23	2:B:182:MET:HG3	1.99	0.45
1:G:7:ILE:HG12	1:G:184:THR:HG23	1.99	0.45
2:F:260:SER:O	2:F:263:THR:OG1	2.35	0.45
2:H:180:VAL:CG2	2:H:272:GLU:HG3	2.47	0.45
2:D:245:GLN:HG2	2:D:248:SER:N	2.32	0.45
1:A:3:LYS:HG2	1:A:160:ALA:HB2	1.98	0.45
1:C:81:THR:HG21	2:D:191:LEU:HD11	1.99	0.45
1:E:195:ASN:C	1:E:195:ASN:HD22	2.19	0.44
2:B:292:ASP:O	2:B:296:MET:HG2	2.18	0.44
2:H:237:GLN:CG	2:H:244:SER:HB3	2.48	0.44
1:E:200:LEU:O	1:E:204:TYR:HD2	2.00	0.44
1:E:131:ILE:O	1:E:132:LEU:HD23	2.17	0.44
2:D:11:ILE:HD12	2:D:12:GLY:O	2.17	0.44
2:D:62:ASN:O	2:D:209:TYR:HE2	2.01	0.44
1:G:12:ALA:HB1	1:G:16:THR:OG1	2.18	0.44
1:E:63:HIS:ND1	1:E:67:ARG:NE	2.66	0.44
1:E:81:THR:HG21	1:E:86:ASP:HB3	1.99	0.44
2:D:18:LEU:HD12	2:F:92:SER:HB3	1.99	0.44
1:G:22:ASP:C	1:G:24:LEU:N	2.71	0.44
1:G:120:GLN:HG2	1:G:121:LEU:N	2.32	0.44
1:G:39:PHE:HB2	1:G:122:ILE:HB	1.99	0.44
1:G:23:ALA:O	1:G:24:LEU:HD12	2.18	0.44
1:G:58:TYR:CD2	1:G:210:LEU:HD13	2.53	0.44
1:A:189:LEU:HD13	1:A:202:TYR:CG	2.53	0.44
1:G:104:ILE:O	1:G:107:ILE:HB	2.18	0.44
1:E:117:MET:HA	1:E:117:MET:CE	2.48	0.44
1:E:37:ILE:HG12	1:E:38:ASP:N	2.33	0.44
1:C:163:PHE:O	1:C:167:ILE:CD1	2.62	0.43
2:B:3:GLN:HB3	2:B:259:VAL:HG22	2.00	0.43
2:F:267:ARG:O	2:F:270:TYR:HB3	2.18	0.43
2:H:3:GLN:OE1	2:H:182:MET:SD	2.76	0.43
1:C:163:PHE:O	1:C:166:LYS:HB2	2.18	0.43
2:D:83:LYS:O	2:D:84:PRO:C	2.55	0.43
2:B:280:LYS:O	2:B:283:GLN:HG2	2.18	0.43
2:F:31:PRO:HB3	2:F:222:PHE:CZ	2.53	0.43
2:B:293:ARG:HA	2:B:296:MET:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:ASN:O	2:B:89:ILE:HG13	2.17	0.43
1:A:142:LEU:CD1	1:A:149:LYS:HD3	2.48	0.43
1:E:25:SER:C	1:E:27:SER:N	2.71	0.43
1:E:32:ARG:CD	1:E:131:ILE:HD11	2.48	0.43
1:E:67:ARG:CD	1:E:67:ARG:N	2.80	0.43
2:B:78:GLU:C	2:B:78:GLU:OE2	2.57	0.43
2:F:29:ASN:HB3	2:F:30:PRO:HD2	2.01	0.43
2:B:30:PRO:HB3	2:D:85:LEU:HG	2.00	0.43
2:B:5:LEU:HD22	2:B:180:VAL:HG23	2.01	0.43
1:A:68:GLN:OE1	1:A:86:ASP:OD2	2.36	0.43
2:H:16:TYR:O	2:H:20:ILE:HG12	2.19	0.43
1:G:162:GLU:O	1:G:166:LYS:HG2	2.19	0.43
2:D:178:ARG:CG	2:D:182:MET:HE3	2.42	0.42
1:E:46:ILE:HG12	2:F:47:TYR:CD2	2.54	0.42
2:H:272:GLU:O	2:H:276:MET:HG2	2.19	0.42
2:B:228:LEU:HA	2:B:257:ILE:HG12	2.00	0.42
1:G:119:ARG:O	1:G:120:GLN:HB2	2.19	0.42
2:H:44:ASN:HB3	2:H:47:TYR:CE2	2.54	0.42
2:B:90:LEU:CD1	2:B:219:GLY:HA2	2.49	0.42
2:F:163:PRO:HA	2:F:190:ILE:O	2.19	0.42
2:D:89:ILE:HG13	2:D:89:ILE:H	1.58	0.42
1:E:201:ALA:O	1:E:205:VAL:HG23	2.20	0.42
1:G:10:GLU:OE1	1:G:10:GLU:CA	2.67	0.42
2:F:26:ILE:HG22	2:F:224:MET:HE1	2.00	0.42
2:B:86:ASN:N	2:B:89:ILE:CD1	2.83	0.42
2:H:261:ARG:HD2	2:H:261:ARG:N	2.34	0.42
2:H:2:VAL:HG23	2:H:261:ARG:NH1	2.35	0.42
2:H:5:LEU:HD12	2:H:271:THR:HG22	2.01	0.42
1:G:10:GLU:OE1	1:G:10:GLU:N	2.52	0.42
2:F:166:LEU:C	2:F:166:LEU:HD23	2.39	0.42
2:B:76:ILE:HD13	2:B:85:LEU:HD11	2.01	0.42
1:A:91:LEU:HA	1:A:91:LEU:HD12	1.82	0.42
2:F:263:THR:HG22	2:F:267:ARG:HD3	1.96	0.42
1:E:48:ASN:C	1:E:55:LYS:HZ1	2.23	0.42
1:G:206:ARG:HH11	1:G:206:ARG:CG	2.31	0.42
1:E:39:PHE:HB3	1:E:122:ILE:HG12	2.02	0.42
1:E:35:TRP:CE2	1:E:138:ARG:HB3	2.55	0.42
1:E:38:ASP:HB2	1:E:61:THR:HB	2.01	0.42
2:B:282:LEU:O	2:B:285:TYR:HB2	2.20	0.42
2:F:270:TYR:O	2:F:273:THR:HB	2.19	0.41
1:G:138:ARG:NH2	1:G:156:GLN:NE2	2.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:300:VAL:CG2	2:F:311:LEU:HD13	2.50	0.41
1:A:210:LEU:HA	1:A:210:LEU:HD23	1.90	0.41
1:C:70:VAL:HG21	1:C:197:ILE:HD12	2.01	0.41
2:B:197:ASN:HB3	2:B:202:SER:HB3	2.01	0.41
1:E:40:ARG:HB2	1:E:59:SER:HB3	2.02	0.41
1:G:24:LEU:O	1:G:27:SER:N	2.47	0.41
1:A:39:PHE:HB2	1:A:122:ILE:HG12	2.01	0.41
1:G:37:ILE:HG12	1:G:38:ASP:N	2.35	0.41
1:E:210:LEU:HD23	1:E:210:LEU:O	2.21	0.41
1:E:130:LEU:HB2	1:E:137:VAL:HG23	2.02	0.41
2:F:293:ARG:O	2:F:297:ASP:N	2.46	0.41
2:H:233:GLN:HG2	2:H:252:LEU:O	2.21	0.41
1:G:147:GLY:O	1:G:148:PHE:C	2.59	0.41
2:F:180:VAL:CG1	2:F:272:GLU:HG3	2.51	0.41
2:B:2:VAL:HA	2:B:261:ARG:HD2	2.01	0.41
1:C:160:ALA:O	1:C:161:GLY:C	2.59	0.41
2:D:246:ILE:HG23	2:D:311:LEU:CD2	2.51	0.41
2:H:82:ASP:O	2:H:83:LYS:CE	2.68	0.41
2:H:44:ASN:HB3	2:H:47:TYR:HD2	1.84	0.41
1:E:59:SER:HG	1:E:105:ASP:CG	2.24	0.41
1:E:163:PHE:HA	1:E:166:LYS:HG3	2.03	0.41
2:H:263:THR:OG1	2:H:268:ILE:HD11	2.21	0.41
2:B:5:LEU:HD21	2:B:182:MET:HE2	2.03	0.41
1:E:111:LYS:C	1:E:112:LEU:HD12	2.40	0.41
1:C:40:ARG:HD3	1:C:118:GLN:NE2	2.35	0.41
2:D:293:ARG:O	2:D:295:SER:N	2.50	0.41
2:D:78:GLU:O	2:D:79:THR:HB	2.21	0.40
1:G:164:GLU:H	1:G:164:GLU:HG3	1.68	0.40
2:B:90:LEU:HD21	2:B:218:ILE:HG22	2.03	0.40
1:C:111:LYS:NZ	2:D:170:ASP:OD2	2.50	0.40
2:B:86:ASN:C	2:B:86:ASN:ND2	2.74	0.40
1:G:100:VAL:HG11	2:H:261:ARG:HH12	1.87	0.40
2:D:260:SER:HA	2:D:261:ARG:NH1	2.36	0.40
1:C:100:VAL:HB	2:D:2:VAL:CG2	2.44	0.40
2:H:228:LEU:HA	2:H:257:ILE:HG12	2.03	0.40
1:E:117:MET:HA	1:E:117:MET:HE3	2.03	0.40
1:G:112:LEU:N	1:G:112:LEU:HD12	2.36	0.40
1:C:163:PHE:HA	1:C:166:LYS:CG	2.51	0.40
1:E:46:ILE:HB	1:E:55:LYS:HZ3	1.86	0.40
1:G:159:GLU:HB2	1:G:162:GLU:CD	2.41	0.40
1:C:104:ILE:HD12	1:C:107:ILE:HB	2.04	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	201/212 (95%)	193 (96%)	5 (2%)	3 (2%)	13	17
1	C	189/212 (89%)	172 (91%)	14 (7%)	3 (2%)	12	16
1	E	191/212 (90%)	163 (85%)	23 (12%)	5 (3%)	7	6
1	G	190/212 (90%)	161 (85%)	23 (12%)	6 (3%)	5	4
2	B	217/317 (68%)	209 (96%)	5 (2%)	3 (1%)	14	19
2	D	227/317 (72%)	209 (92%)	14 (6%)	4 (2%)	11	13
2	F	230/317 (73%)	221 (96%)	8 (4%)	1 (0%)	39	56
2	H	216/317 (68%)	195 (90%)	15 (7%)	6 (3%)	6	5
All	All	1661/2116 (78%)	1523 (92%)	107 (6%)	31 (2%)	10	12

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	193	THR
1	C	161	GLY
1	C	187	ASP
2	D	79	THR
1	E	126	ALA
2	F	103	ALA
1	G	10	GLU
2	H	84	PRO
2	B	292	ASP
1	G	133	ASP
1	G	163	PHE
2	D	62	ASN
2	D	294	GLN

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Mol	Chain	Res	Type
1	E	3	LYS
1	E	148	PHE
1	G	25	SER
2	H	302	HIS
2	B	48	ASP
2	B	84	PRO
2	H	62	ASN
2	H	79	THR
2	H	241	ALA
1	C	25	SER
1	G	164	GLU
1	G	176	GLU
2	H	81	MET
1	E	179	ALA
1	E	127	GLY
1	A	191	PRO
2	D	84	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	174/179 (97%)	163 (94%)	11 (6%)	22	35
1	C	166/179 (93%)	158 (95%)	8 (5%)	31	49
1	E	167/179 (93%)	160 (96%)	7 (4%)	36	56
1	G	166/179 (93%)	159 (96%)	7 (4%)	36	56
2	B	204/288 (71%)	192 (94%)	12 (6%)	24	38
2	D	207/288 (72%)	194 (94%)	13 (6%)	22	35
2	F	214/288 (74%)	207 (97%)	7 (3%)	45	66
2	H	203/288 (70%)	196 (97%)	7 (3%)	44	65
All	All	1501/1868 (80%)	1429 (95%)	72 (5%)	31	49

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LEU
1	A	67	ARG
1	A	71	LEU
1	A	91	LEU
1	A	121	LEU
1	A	137	VAL
1	A	142	LEU
1	A	174	LEU
1	A	189	LEU
1	A	192	ASP
1	A	195	ASN
2	B	2	VAL
2	B	18	LEU
2	B	66	LEU
2	B	77	ASP
2	B	78	GLU
2	B	86	ASN
2	B	261	ARG
2	B	275	LEU
2	B	283	GLN
2	B	292	ASP
2	B	307	ILE
2	B	313	HIS
1	C	11	ARG
1	C	71	LEU
1	C	121	LEU
1	C	137	VAL
1	C	178	ARG
1	C	181	GLU
1	C	195	ASN
1	C	197	ILE
2	D	3	GLN
2	D	5	LEU
2	D	11	ILE
2	D	18	LEU
2	D	70	VAL
2	D	72	PHE
2	D	80	MET
2	D	86	ASN
2	D	177	ASN
2	D	261	ARG
2	D	266	ASP
2	D	275	LEU

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Mol	Chain	Res	Type
2	D	307	ILE
1	E	56	LEU
1	E	57	MET
1	E	121	LEU
1	E	125	ASP
1	E	152	LEU
1	E	195	ASN
1	E	209	GLU
2	F	18	LEU
2	F	72	PHE
2	F	79	THR
2	F	91	LYS
2	F	102	TYR
2	F	200	VAL
2	F	261	ARG
1	G	10	GLU
1	G	11	ARG
1	G	162	GLU
1	G	178	ARG
1	G	189	LEU
1	G	197	ILE
1	G	210	LEU
2	H	66	LEU
2	H	76	ILE
2	H	82	ASP
2	H	84	PRO
2	H	95	ASN
2	H	240	GLU
2	H	261	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	68	GLN
1	A	114	ASN
1	A	118	GLN
2	B	3	GLN
2	B	86	ASN
2	B	183	GLN
2	B	205	ASN
2	B	258	ASN

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Mol	Chain	Res	Type
2	B	269	ASN
2	B	283	GLN
2	B	294	GLN
2	B	313	HIS
1	C	63	HIS
1	C	68	GLN
1	C	94	ASN
1	C	118	GLN
1	C	195	ASN
2	D	3	GLN
2	D	86	ASN
2	D	176	ASN
2	D	177	ASN
2	D	183	GLN
2	D	197	ASN
2	D	205	ASN
2	D	258	ASN
2	D	294	GLN
1	E	68	GLN
1	E	118	GLN
1	E	120	GLN
1	E	195	ASN
2	F	101	ASN
2	F	237	GLN
2	F	258	ASN
1	G	65	HIS
1	G	68	GLN
1	G	118	GLN
1	G	120	GLN
1	G	156	GLN
1	G	195	ASN
2	H	3	GLN
2	H	95	ASN
2	H	167	GLN
2	H	183	GLN
2	H	237	GLN
2	H	258	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
3	PO4	A	211	-	4,4,4	1.10	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
3	PO4	A	211	-	-	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.

No monomer is involved in short contacts.

## 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	205/212 (96%)	-0.09	6 (2%) 55 54	20, 31, 57, 91	0
1	C	195/212 (91%)	0.50	19 (9%) 10 9	29, 58, 84, 91	0
1	E	197/212 (92%)	1.43	55 (27%) 1 1	30, 88, 100, 100	0
1	G	196/212 (92%)	1.58	66 (33%) 0 0	36, 91, 100, 100	0
2	B	227/317 (71%)	0.11	15 (6%) 22 22	20, 39, 71, 94	0
2	D	233/317 (73%)	0.35	21 (9%) 12 11	24, 45, 82, 91	0
2	F	238/317 (75%)	0.11	14 (5%) 26 26	21, 43, 77, 95	0
2	H	226/317 (71%)	0.98	46 (20%) 1 1	35, 74, 99, 100	0
All	All	1717/2116 (81%)	0.60	242 (14%) 4 4	20, 55, 99, 100	0

All (242) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	160	ALA	12.7
1	G	2	GLY	10.4
1	G	160	ALA	9.9
2	H	262	GLY	7.4
1	G	65	HIS	7.3
2	F	171	ILE	6.6
1	E	210	LEU	6.6
1	G	134	GLY	6.4
1	C	46	ILE	6.3
1	G	63	HIS	6.2
2	H	300	VAL	6.2
2	B	50	GLU	6.2
1	C	65	HIS	6.1
1	E	30	SER	5.9
2	H	265	ILE	5.9
2	H	241	ALA	5.9

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Mol	Chain	Res	Type	RSRZ
2	H	81	MET	5.8
1	E	158	ASP	5.8
1	E	65	HIS	5.7
2	H	82	ASP	5.6
2	H	243	ASN	5.4
2	H	47	TYR	5.3
1	G	46	ILE	5.2
2	B	293	ARG	5.2
1	G	161	GLY	5.2
1	G	66	GLY	5.0
1	G	71	LEU	4.9
2	D	299	ARG	4.8
1	E	153	ILE	4.8
2	F	104	MET	4.8
1	E	64	HIS	4.7
1	G	146	THR	4.7
2	H	261	ARG	4.7
1	G	55	LYS	4.7
1	G	29	LEU	4.6
1	E	161	GLY	4.6
1	E	26	ASN	4.6
2	H	296	MET	4.5
2	D	160	SER	4.5
2	H	242	GLY	4.4
1	G	39	PHE	4.4
2	D	241	ALA	4.4
2	F	103	ALA	4.4
2	H	61	PRO	4.3
2	H	45	PRO	4.3
2	D	242	GLY	4.2
1	E	2	GLY	4.2
2	D	240	GLU	4.2
2	D	173	ALA	4.2
2	D	82	ASP	4.1
2	F	262	GLY	4.1
1	E	159	GLU	4.1
1	E	176	GLU	4.1
2	D	174	ALA	4.0
2	H	79	THR	4.0
1	G	178	ARG	4.0
1	G	64	HIS	4.0
1	G	159	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
2	H	78	GLU	4.0
1	G	67	ARG	4.0
1	G	59	SER	3.9
1	G	119	ARG	3.8
2	B	240	GLU	3.8
1	G	145	SER	3.8
1	E	33	ASP	3.8
1	E	47	LYS	3.8
1	G	43	ARG	3.7
1	E	48	ASN	3.7
1	G	44	CYS	3.7
2	F	159	GLU	3.7
2	D	77	ASP	3.7
1	E	140	VAL	3.7
1	E	55	LYS	3.7
1	G	28	ILE	3.6
1	C	153	ILE	3.5
1	A	191	PRO	3.5
2	H	46	SER	3.5
1	G	56	LEU	3.5
2	H	80	MET	3.5
1	E	152	LEU	3.5
1	G	133	ASP	3.4
1	C	54	SER	3.4
1	A	49	LEU	3.4
2	H	170	ASP	3.4
1	G	132	LEU	3.4
2	D	196	LYS	3.4
1	C	11	ARG	3.4
1	E	178	ARG	3.4
2	F	46	SER	3.3
2	H	295	SER	3.3
1	G	75	ASN	3.3
2	H	95	ASN	3.3
1	C	181	GLU	3.3
1	G	196	GLU	3.3
1	C	55	LYS	3.3
2	H	196	LYS	3.3
1	E	34	PRO	3.3
1	E	157	ALA	3.3
1	A	48	ASN	3.3
2	F	313	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
1	G	195	ASN	3.3
1	C	71	LEU	3.2
1	C	119	ARG	3.2
2	F	261	ARG	3.2
1	G	11	ARG	3.2
1	E	27	SER	3.2
1	E	29	LEU	3.2
1	E	131	ILE	3.2
1	G	164	GLU	3.2
1	G	176	GLU	3.2
2	H	240	GLU	3.1
1	E	43	ARG	3.1
1	G	152	LEU	3.1
2	D	47	TYR	3.1
2	H	297	ASP	3.1
2	B	294	GLN	3.1
2	F	265	ILE	3.1
1	G	144	SER	3.1
2	H	280	LYS	3.1
2	H	267	ARG	3.1
1	C	162	GLU	3.0
2	H	291	PRO	3.0
1	E	180	LYS	3.0
1	C	66	GLY	3.0
1	E	32	ARG	3.0
2	D	78	GLU	3.0
1	E	67	ARG	3.0
1	G	32	ARG	3.0
1	A	193	THR	2.9
1	E	31	VAL	2.9
1	E	133	ASP	2.9
1	G	34	PRO	2.9
1	E	123	LYS	2.9
1	G	180	LYS	2.9
1	E	22	ASP	2.8
1	G	33	ASP	2.8
1	G	58	TYR	2.8
2	H	249	GLY	2.8
2	H	83	LYS	2.8
1	G	209	GLU	2.8
1	E	11	ARG	2.8
1	C	159	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	E	28	ILE	2.7
2	B	83	LYS	2.7
2	B	262	GLY	2.7
2	F	196	LYS	2.7
1	G	3	LYS	2.7
1	C	64	HIS	2.7
1	C	43	ARG	2.7
2	B	49	VAL	2.7
2	B	159	GLU	2.7
1	G	163	PHE	2.7
1	E	138	ARG	2.6
2	B	48	ASP	2.6
2	D	46	SER	2.6
2	H	171	ILE	2.6
1	E	117	MET	2.6
2	B	74	TYR	2.5
1	E	134	GLY	2.5
1	C	196	GLU	2.5
1	E	145	SER	2.5
2	D	294	GLN	2.5
1	E	74	ASP	2.5
2	H	287	GLU	2.5
1	G	31	VAL	2.5
1	E	146	THR	2.5
1	E	66	GLY	2.5
1	G	157	ALA	2.5
2	F	45	PRO	2.5
2	B	292	ASP	2.5
1	G	117	MET	2.5
2	H	299	ARG	2.4
2	H	263	THR	2.4
1	C	26	ASN	2.4
2	H	239	GLU	2.4
2	D	172	PRO	2.4
1	G	60	ILE	2.4
2	B	77	ASP	2.4
2	H	3	GLN	2.4
1	E	15	ALA	2.4
1	E	162	GLU	2.4
2	F	74	TYR	2.4
1	E	128	GLU	2.4
2	H	269	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	143	PHE	2.3
2	F	293	ARG	2.3
2	H	270	TYR	2.3
1	G	24	LEU	2.3
2	D	297	ASP	2.3
2	H	74	TYR	2.3
2	D	45	PRO	2.3
1	G	154	GLU	2.3
1	E	148	PHE	2.3
2	H	290	VAL	2.3
1	G	173	HIS	2.3
1	C	63	HIS	2.3
2	H	313	HIS	2.3
2	D	74	TYR	2.3
2	F	102	TYR	2.3
2	H	197	ASN	2.2
1	E	155	LEU	2.2
1	G	168	ALA	2.2
1	E	62	PHE	2.2
2	H	284	GLY	2.2
1	E	71	LEU	2.2
1	C	146	THR	2.2
1	G	138	ARG	2.2
1	E	39	PHE	2.2
1	G	123	LYS	2.2
1	G	158	ASP	2.2
1	E	179	ALA	2.2
2	B	287	GLU	2.2
2	H	14	ASP	2.2
1	G	131	ILE	2.1
1	G	62	PHE	2.1
2	H	253	LEU	2.1
2	D	84	PRO	2.1
2	D	298	SER	2.1
1	G	187	ASP	2.1
1	G	30	SER	2.1
1	A	189	LEU	2.1
1	G	189	LEU	2.1
2	B	313	HIS	2.1
1	A	192	ASP	2.1
1	G	37	ILE	2.1
1	E	75	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
2	H	283	GLN	2.1
1	G	17	LEU	2.1
2	H	91	LYS	2.1
1	G	210	LEU	2.1
2	H	211	PHE	2.1
1	E	5	ALA	2.0
1	G	23	ALA	2.0
1	E	46	ILE	2.0
2	B	7	LEU	2.0
1	C	59	SER	2.0
1	E	59	SER	2.0
1	G	109	SER	2.0
2	D	79	THR	2.0
1	E	207	ALA	2.0
1	G	174	LEU	2.0
1	G	61	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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
3	PO4	A	211	5/5	0.99	0.10	-1.27	43,44,47,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.