



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 19, 2026 – 08:30 PM UTC

PDB ID : 7OZ2 / pdb_00007oz2
Title : Crystal structure of HIV-1 reverse transcriptase with a double stranded DNA showing a transient P-pocket
Authors : Martinez, S.E.; Singh, A.K.; Das, K.
Deposited on : 2021-06-25
Resolution : 2.85 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

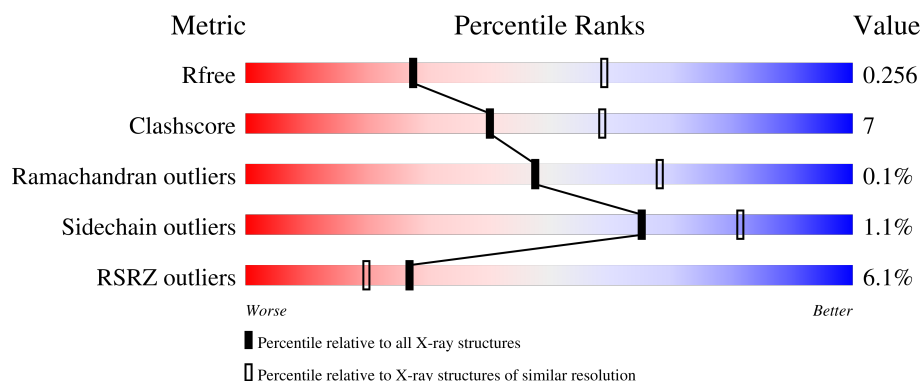
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	556	2% 83% 16%
1	C	556	8% 78% 21% ..
2	B	444	5% 79% 15% 6%
2	D	444	9% 74% 17% 9%
3	E	28	11% 46% 39% 14%

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Mol	Chain	Length	Quality of chain
3	T	28	 75% 14% 11%
4	F	21	 5% 76% 24%
4	P	21	 62% 38%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17868 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 Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4514	2921	751	834	8			
1	C	551	Total	C	N	O	S	0	0	0
			4486	2902	747	829	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP P03366
A	0	VAL	-	expression tag	UNP P03366
A	63	CYS	ILE	conflict	UNP P03366
A	280	SER	CYS	conflict	UNP P03366
C	-1	MET	-	initiating methionine	UNP P03366
C	0	VAL	-	expression tag	UNP P03366
C	63	CYS	ILE	conflict	UNP P03366
C	280	SER	CYS	conflict	UNP P03366

- Molecule 2 is a protein called Gag-Pol polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	417	Total	C	N	O	S	0	0	0
			3449	2246	573	623	7			
2	D	406	Total	C	N	O	S	0	0	0
			3355	2185	552	611	7			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	MET	-	initiating methionine	UNP P03366
B	-14	ALA	-	expression tag	UNP P03366
B	-13	HIS	-	expression tag	UNP P03366
B	-12	HIS	-	expression tag	UNP P03366

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	HIS	-	expression tag	UNP P03366
B	-10	HIS	-	expression tag	UNP P03366
B	-9	HIS	-	expression tag	UNP P03366
B	-8	HIS	-	expression tag	UNP P03366
B	-7	ALA	-	expression tag	UNP P03366
B	-6	LEU	-	expression tag	UNP P03366
B	-5	GLU	-	expression tag	UNP P03366
B	-4	VAL	-	expression tag	UNP P03366
B	-3	LEU	-	expression tag	UNP P03366
B	-2	PHE	-	expression tag	UNP P03366
B	-1	GLN	-	expression tag	UNP P03366
B	0	GLY	-	expression tag	UNP P03366
B	280	SER	CYS	engineered mutation	UNP P03366
D	-15	MET	-	initiating methionine	UNP P03366
D	-14	ALA	-	expression tag	UNP P03366
D	-13	HIS	-	expression tag	UNP P03366
D	-12	HIS	-	expression tag	UNP P03366
D	-11	HIS	-	expression tag	UNP P03366
D	-10	HIS	-	expression tag	UNP P03366
D	-9	HIS	-	expression tag	UNP P03366
D	-8	HIS	-	expression tag	UNP P03366
D	-7	ALA	-	expression tag	UNP P03366
D	-6	LEU	-	expression tag	UNP P03366
D	-5	GLU	-	expression tag	UNP P03366
D	-4	VAL	-	expression tag	UNP P03366
D	-3	LEU	-	expression tag	UNP P03366
D	-2	PHE	-	expression tag	UNP P03366
D	-1	GLN	-	expression tag	UNP P03366
D	0	GLY	-	expression tag	UNP P03366
D	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 3 is a DNA chain called DNA (28-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	T	25	Total	C	N	O	P	0	0	0
			517	243	102	147	25			
3	E	24	Total	C	N	O	P	0	0	0
			496	233	97	142	24			

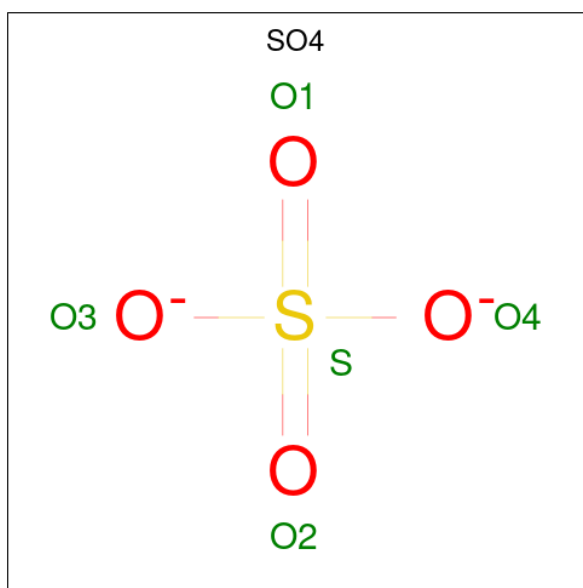
- Molecule 4 is a DNA chain called DNA (5'-D(*AP*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*GP*CP*GP*CP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	P	21	Total 425	C 202	N 77	O 126	P 20	0	0	0
4	F	21	Total 428	C 202	N 77	O 128	P 21	0	0	0

- Molecule 5 is CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	7	Total 7	Cd 7	0	0
5	B	3	Total 3	Cd 3	0	0
5	T	4	Total 4	Cd 4	0	0
5	P	2	Total 2	Cd 2	0	0
5	C	3	Total 3	Cd 3	0	0
5	D	3	Total 3	Cd 3	0	0
5	E	3	Total 3	Cd 3	0	0
5	F	2	Total 2	Cd 2	0	0

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Mg	0	0
			1	1		

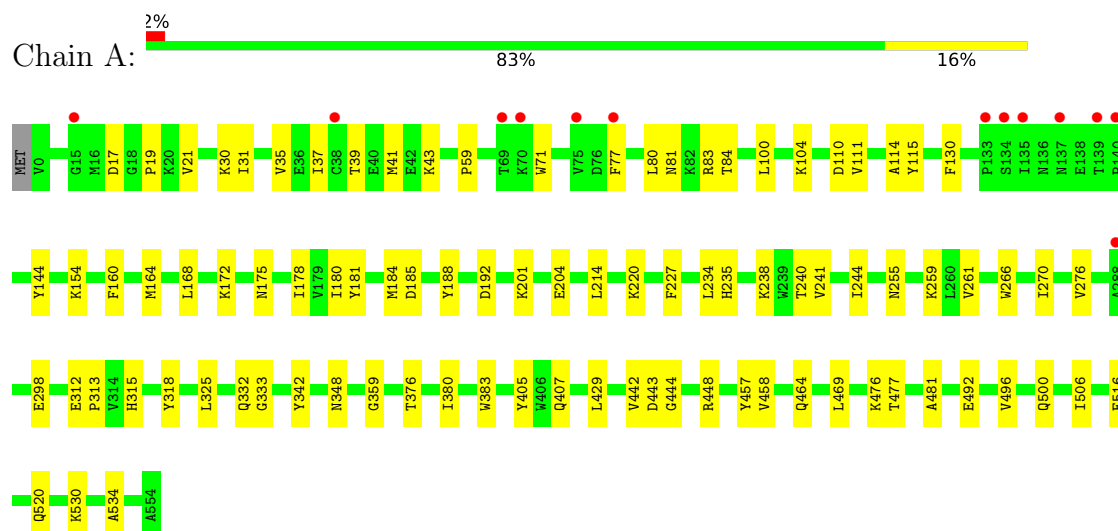
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	55	Total	O	0	0
			55	55		
8	B	43	Total	O	0	0
			43	43		
8	T	6	Total	O	0	0
			6	6		
8	P	6	Total	O	0	0
			6	6		
8	C	20	Total	O	0	0
			20	20		
8	D	25	Total	O	0	0
			25	25		
8	E	4	Total	O	0	0
			4	4		
8	F	1	Total	O	0	0
			1	1		

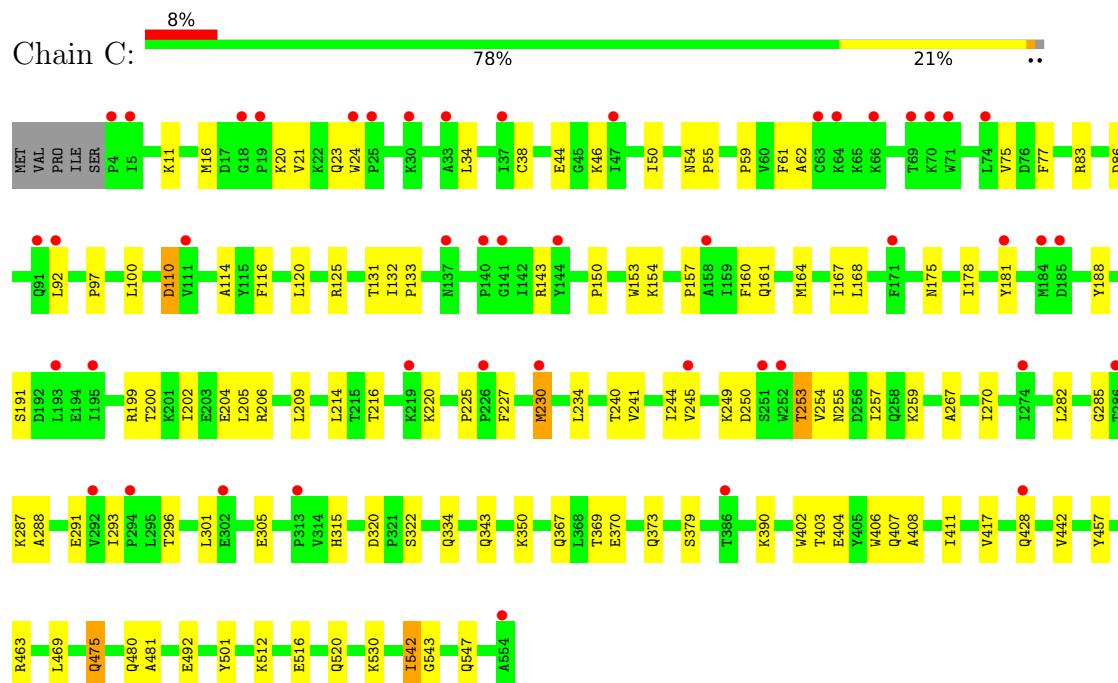
3 Residue-property plots [i](#)

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.

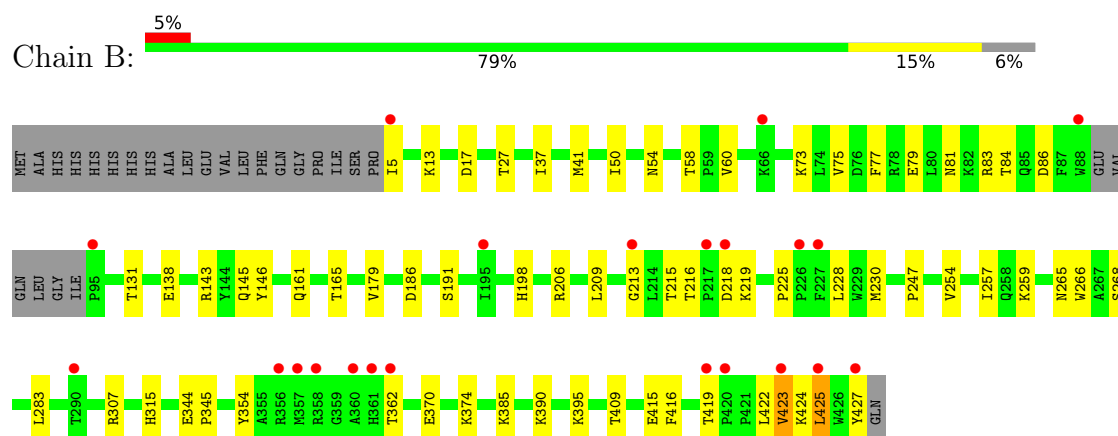
- Molecule 1: Reverse transcriptase/ribonuclease H



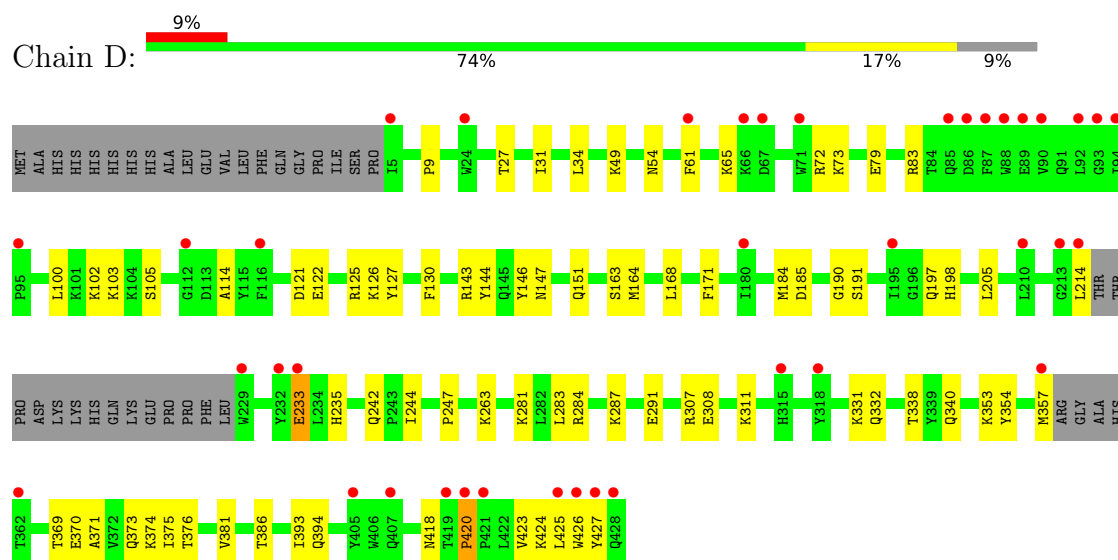
- Molecule 1: Reverse transcriptase/ribonuclease H



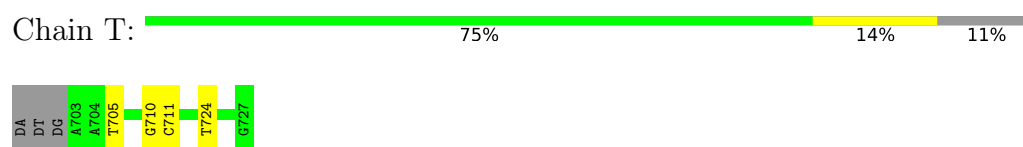
- Molecule 2: Gag-Pol polyprotein



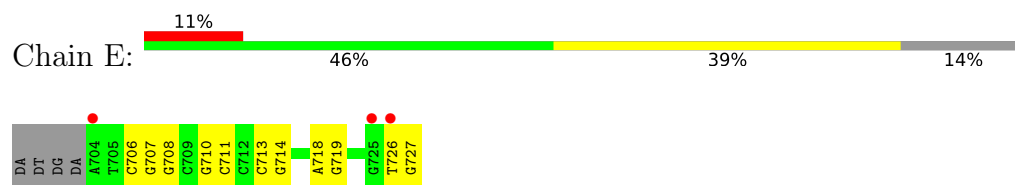
- Molecule 2: Gag-Pol polyprotein



- Molecule 3: DNA (28-MER)

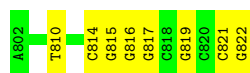


- Molecule 3: DNA (28-MER)



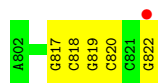
- Molecule 4: DNA (5'-D(*AP*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*GP*CP*GP*CP*CP*G)-3')

Chain P:  62% 38%



- Molecule 4: DNA (5'-D(*AP*CP*AP*GP*TP*CP*CP*CP*TP*GP*TP*TP*CP*GP*GP*GP*CP*GP*CP*CP*G)-3')

Chain F:  5% 76% 24%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	310.64Å 62.07Å 168.24Å 90.00° 104.51° 90.00°	Depositor
Resolution (Å)	81.44 – 2.85 81.44 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.7 (81.44-2.85) 99.7 (81.44-2.85)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.217 , 0.257 0.216 , 0.256	Depositor DCC
R_{free} test set	3706 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	56.9	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17868	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.17	0/4632	0.32	0/6294
1	C	0.19	0/4603	0.38	4/6252 (0.1%)
2	B	0.16	0/3550	0.34	1/4822 (0.0%)
2	D	0.21	0/3448	0.39	1/4681 (0.0%)
3	E	0.34	0/557	0.57	0/858
3	T	0.30	0/581	0.41	0/895
4	F	0.35	0/478	0.56	0/735
4	P	0.35	0/475	0.58	0/731
All	All	0.21	0/18324	0.38	6/25268 (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	D	420	PRO	N-CA-C	10.95	124.05	110.70
1	C	543	GLY	N-CA-C	6.74	129.15	113.18
1	C	270	ILE	CB-CA-C	5.71	120.65	111.29
1	C	542	ILE	N-CA-C	5.65	116.08	108.17
2	B	423	VAL	N-CA-C	-5.51	97.87	109.34
1	C	230	MET	N-CA-C	5.44	119.08	111.74

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	4514	0	4573	61	0
1	C	4486	0	4539	74	0
2	B	3449	0	3480	41	0
2	D	3355	0	3386	47	0
3	E	496	0	268	6	0
3	T	517	0	279	4	0
4	F	428	0	236	5	0
4	P	425	0	237	8	0
5	A	7	0	0	0	0
5	B	3	0	0	0	0
5	C	3	0	0	0	0
5	D	3	0	0	0	0
5	E	3	0	0	0	0
5	F	2	0	0	0	0
5	P	2	0	0	0	0
5	T	4	0	0	0	0
6	A	5	0	0	0	0
6	B	5	0	0	1	0
7	C	1	0	0	0	0
8	A	55	0	0	1	0
8	B	43	0	0	3	0
8	C	20	0	0	0	0
8	D	25	0	0	0	0
8	E	4	0	0	0	0
8	F	1	0	0	0	0
8	P	6	0	0	1	0
8	T	6	0	0	0	0
All	All	17868	0	16998	229	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 7.

All (229) 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:164:MET:HE3	1:C:168:LEU:HD21	1.53	0.88
3:E:706:DC:H2'	3:E:707:DG:C8	2.18	0.77
1:C:475:GLN:H	1:C:475:GLN:NE2	1.83	0.76
1:C:475:GLN:H	1:C:475:GLN:HE21	1.34	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:LYS:NZ	1:A:204:GLU:OE1	2.21	0.70
2:B:225:PRO:HG2	2:B:228:LEU:HB2	1.72	0.70
2:B:424:LYS:NZ	2:B:427:TYR:O	2.24	0.70
1:A:184:MET:HG2	4:P:821:DC:H2''	1.74	0.69
2:D:125:ARG:HD3	2:D:146:TYR:O	1.92	0.68
2:B:259:LYS:NZ	8:B:601:HOH:O	2.27	0.67
2:B:206:ARG:NH1	2:B:216:THR:O	2.28	0.67
2:B:354:TYR:CE2	2:B:374:LYS:HB2	2.30	0.67
2:B:79:GLU:HG3	2:B:83:ARG:HE	1.60	0.65
1:C:206:ARG:NH2	1:C:216:THR:O	2.29	0.65
1:C:209:LEU:HB3	1:C:214:LEU:HB2	1.79	0.65
2:B:230:MET:HE1	2:B:370:GLU:HG2	1.80	0.64
2:D:151:GLN:HB3	2:D:185:ASP:OD2	1.98	0.63
1:A:227:PHE:HB2	1:A:234:LEU:HB2	1.80	0.63
2:B:354:TYR:HE2	2:B:374:LYS:HB2	1.63	0.63
1:C:390:LYS:HE3	1:C:417:VAL:HG11	1.81	0.63
1:C:199:ARG:HA	1:C:202:ILE:HB	1.80	0.62
1:A:261:VAL:HG13	1:A:276:VAL:HG21	1.81	0.62
1:C:120:LEU:HD23	1:C:125:ARG:HG2	1.80	0.62
1:C:86:ASP:OD1	1:C:154:LYS:NZ	2.29	0.62
1:A:448:ARG:NH2	3:T:724:DT:O2	2.32	0.62
1:A:104:LYS:HB2	1:A:192:ASP:HA	1.81	0.62
1:C:288:ALA:HB3	1:C:291:GLU:HB2	1.81	0.62
2:D:287:LYS:NZ	2:D:291:GLU:OE2	2.33	0.61
1:A:516:GLU:CD	1:A:516:GLU:H	2.08	0.61
2:B:73:LYS:NZ	2:B:146:TYR:OH	2.29	0.60
2:B:247:PRO:O	2:B:307:ARG:NH2	2.34	0.60
1:C:16:MET:HE2	1:C:83:ARG:HG3	1.84	0.60
2:B:385:LYS:NZ	8:B:604:HOH:O	2.35	0.59
2:D:354:TYR:HB3	2:D:357:MET:HE3	1.85	0.59
1:C:369:THR:HG22	1:C:411:ILE:HD11	1.85	0.59
3:E:726:DT:H2''	3:E:727:DG:H5'	1.84	0.58
1:C:164:MET:O	1:C:167:ILE:N	2.37	0.58
2:D:338:THR:HG21	2:D:427:TYR:HB2	1.86	0.58
1:C:254:VAL:HG23	1:C:293:ILE:HD11	1.84	0.57
2:D:65:LYS:HE2	2:D:72:ARG:HD2	1.86	0.57
1:C:457:TYR:HE1	1:C:463:ARG:HG2	1.68	0.57
2:B:266:TRP:CD2	2:B:425:LEU:HD13	2.39	0.57
1:C:44:GLU:OE1	1:C:46:LYS:NZ	2.38	0.57
1:A:172:LYS:HG2	1:A:180:ILE:HD12	1.87	0.56
2:B:254:VAL:HG13	2:B:283:LEU:HD22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:ILE:HD11	1:A:71:TRP:HB2	1.87	0.55
1:C:282:LEU:HD22	1:C:296:THR:HG23	1.88	0.55
1:A:238:LYS:HE3	1:A:315:HIS:CD2	2.42	0.55
1:C:285:GLY:O	1:C:287:LYS:NZ	2.33	0.55
2:D:54:ASN:HB3	2:D:143:ARG:HH21	1.71	0.55
2:D:114:ALA:HB2	2:D:214:LEU:HD13	1.88	0.55
1:A:164:MET:HE2	1:A:168:LEU:HG	1.88	0.55
1:C:54:ASN:O	1:C:143:ARG:NH1	2.41	0.54
4:F:817:DG:H2'	4:F:818:DC:C6	2.42	0.54
1:A:298:GLU:N	1:A:298:GLU:OE1	2.39	0.54
1:C:255:ASN:O	1:C:259:LYS:HG2	2.08	0.54
1:A:380:ILE:HD12	2:B:27:THR:HG22	1.90	0.53
1:C:175:ASN:HB3	1:C:178:ILE:HG12	1.90	0.53
2:D:263:LYS:HA	2:D:425:LEU:HD22	1.90	0.53
1:A:443:ASP:OD1	1:A:444:GLY:N	2.39	0.53
1:C:370:GLU:HG2	2:D:394:GLN:HE22	1.72	0.53
2:D:130:PHE:CZ	2:D:144:TYR:HB2	2.43	0.53
2:D:376:THR:HG23	2:D:386:THR:HG22	1.90	0.53
4:F:818:DC:H2'	4:F:819:DG:C8	2.43	0.53
2:B:81:ASN:ND2	8:B:606:HOH:O	2.40	0.53
2:D:34:LEU:HD11	2:D:61:PHE:HA	1.91	0.53
2:D:242:GLN:HG3	2:D:353:LYS:HE3	1.90	0.53
2:D:371:ALA:O	2:D:375:ILE:HG13	2.09	0.52
1:A:500:GLN:HG2	2:B:422:LEU:HD12	1.92	0.52
1:C:402:TRP:O	2:D:331:LYS:NZ	2.32	0.52
2:D:357:MET:HG2	2:D:374:LYS:NZ	2.25	0.52
1:C:160:PHE:CE1	1:C:164:MET:HG3	2.45	0.52
1:A:458:VAL:HG12	1:A:464:GLN:HG2	1.92	0.52
2:B:54:ASN:HB3	2:B:143:ARG:HH21	1.74	0.51
1:C:320:ASP:O	1:C:343:GLN:NE2	2.38	0.51
2:D:79:GLU:O	2:D:83:ARG:HG3	2.11	0.51
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.93	0.51
2:B:161:GLN:HE21	2:B:165:THR:HG23	1.76	0.51
1:A:19:PRO:HG3	1:A:80:LEU:HB2	1.92	0.51
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.93	0.50
4:P:815:DG:H2'	4:P:816:DG:C8	2.45	0.50
1:A:376:THR:O	1:A:380:ILE:HG12	2.12	0.50
1:C:542:ILE:HG23	2:D:283:LEU:HD13	1.93	0.50
1:A:240:THR:HB	1:A:315:HIS:CD2	2.46	0.50
1:C:24:TRP:HZ2	1:C:61:PHE:HB3	1.77	0.50
2:D:233:GLU:OE2	2:D:235:HIS:NE2	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:VAL:HG11	1:A:244:ILE:HD11	1.94	0.50
2:D:126:LYS:HE3	2:D:127:TYR:CZ	2.46	0.49
2:D:191:SER:OG	2:D:198:HIS:ND1	2.28	0.49
1:A:110:ASP:HB3	1:A:220:LYS:HB3	1.94	0.49
2:B:315:HIS:NE2	6:B:504:SO4:O4	2.44	0.49
1:A:359:GLY:HA2	4:P:810:DT:OP2	2.12	0.49
1:C:23:GLN:HG2	1:C:133:PRO:HD3	1.95	0.49
1:C:131:THR:HG22	1:C:143:ARG:HG3	1.94	0.49
1:A:111:VAL:HB	1:A:185:ASP:HB2	1.94	0.49
1:A:405:TYR:CE2	1:A:407:GLN:HB2	2.47	0.49
1:C:50:ILE:HG13	1:C:143:ARG:HD2	1.94	0.49
2:D:100:LEU:HG	2:D:381:VAL:HG13	1.94	0.49
1:C:492:GLU:HG2	1:C:530:LYS:HB2	1.95	0.49
1:A:312:GLU:OE2	1:A:313:PRO:HD2	2.13	0.49
1:C:369:THR:O	1:C:373:GLN:HG3	2.12	0.49
1:A:19:PRO:HD3	1:A:80:LEU:HD13	1.95	0.49
1:A:21:VAL:HB	1:A:59:PRO:HD3	1.95	0.49
2:D:103:LYS:HZ2	2:D:191:SER:HA	1.77	0.49
1:C:253:THR:O	1:C:257:ILE:HG12	2.13	0.48
2:B:390:LYS:NZ	2:B:415:GLU:OE2	2.45	0.48
2:D:122:GLU:HA	2:D:125:ARG:HG3	1.94	0.48
1:C:20:LYS:HZ1	1:C:55:PRO:HG2	1.77	0.48
1:C:178:ILE:HD12	1:C:191:SER:HB2	1.96	0.48
1:A:469:LEU:HD12	1:A:477:THR:HG22	1.96	0.48
1:C:181:TYR:HB2	1:C:188:TYR:HB3	1.96	0.48
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.94	0.48
2:D:247:PRO:O	2:D:307:ARG:NH2	2.43	0.47
2:D:332:GLN:HG3	2:D:338:THR:HG23	1.96	0.47
4:P:817:DG:N7	8:P:1001:HOH:O	2.35	0.47
1:A:84:THR:HB	1:A:154:LYS:HE2	1.95	0.47
2:B:50:ILE:HD13	2:B:145:GLN:HB3	1.96	0.47
2:B:344:GLU:HG3	2:B:345:PRO:HD2	1.97	0.47
1:C:20:LYS:HZ2	1:C:55:PRO:C	2.23	0.47
1:C:200:THR:O	1:C:204:GLU:HG3	2.14	0.47
1:A:17:ASP:O	1:A:83:ARG:HD3	2.15	0.47
1:C:110:ASP:HB2	1:C:220:LYS:HB3	1.97	0.47
2:D:9:PRO:HA	2:D:121:ASP:OD2	2.15	0.47
1:C:21:VAL:HB	1:C:59:PRO:HD3	1.97	0.46
1:C:320:ASP:OD1	1:C:322:SER:OG	2.30	0.46
1:C:240:THR:OG1	1:C:315:HIS:HA	2.15	0.46
1:C:249:LYS:HG2	1:C:250:ASP:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:516:GLU:O	1:C:520:GLN:HG3	2.16	0.46
1:C:403:THR:OG1	1:C:404:GLU:OE1	2.32	0.46
2:D:73:LYS:HE2	2:D:146:TYR:OH	2.14	0.46
2:D:340:GLN:HG2	2:D:426:TRP:CH2	2.50	0.46
1:A:39:THR:O	1:A:43:LYS:HG3	2.15	0.46
1:A:342:TYR:HB3	1:A:348:ASN:HA	1.97	0.46
1:C:442:VAL:HG12	1:C:457:TYR:HB3	1.98	0.46
1:A:332:GLN:HG3	1:A:333:GLY:H	1.81	0.46
1:C:241:VAL:HG21	1:C:244:ILE:HD11	1.96	0.46
1:A:30:LYS:NZ	3:T:705:DT:O4	2.39	0.46
1:A:37:ILE:O	1:A:41:MET:HG2	2.15	0.46
2:B:206:ARG:NH2	2:B:218:ASP:HB3	2.30	0.46
1:A:35:VAL:O	1:A:39:THR:HG23	2.16	0.45
2:B:206:ARG:HD2	2:B:215:THR:HG21	1.98	0.45
1:A:325:LEU:HD21	1:A:383:TRP:CE3	2.51	0.45
1:C:150:PRO:HG2	1:C:153:TRP:HB2	1.97	0.45
1:C:475:GLN:HB3	1:C:501:TYR:CE2	2.51	0.45
2:B:17:ASP:O	2:B:83:ARG:HD3	2.17	0.45
2:D:308:GLU:HA	2:D:311:LYS:HE2	1.98	0.45
1:C:475:GLN:NE2	1:C:475:GLN:N	2.61	0.45
1:C:34:LEU:HD21	1:C:62:ALA:HB2	1.98	0.45
1:C:442:VAL:HB	1:C:481:ALA:HB1	1.98	0.45
1:A:111:VAL:HG11	1:A:214:LEU:HD22	1.98	0.45
1:A:492:GLU:HG2	1:A:530:LYS:HB2	1.99	0.45
2:B:370:GLU:O	2:B:374:LYS:HG3	2.16	0.45
1:A:429:LEU:HD11	1:A:506:ILE:HG22	1.98	0.45
3:E:713:DC:H2'	3:E:714:DG:C8	2.52	0.45
2:B:209:LEU:O	2:B:213:GLY:N	2.51	0.44
1:A:448:ARG:HH21	3:T:724:DT:H1'	1.82	0.44
1:A:516:GLU:O	1:A:520:GLN:HG3	2.17	0.44
1:A:181:TYR:CD1	2:B:138:GLU:HG3	2.52	0.44
1:A:266:TRP:CE2	4:P:819:DG:H4'	2.52	0.44
2:B:131:THR:OG1	2:B:143:ARG:HG2	2.16	0.44
1:C:259:LYS:HE3	4:F:820:DC:OP1	2.18	0.44
1:A:114:ALA:HB1	1:A:160:PHE:CZ	2.52	0.44
2:B:265:ASN:O	2:B:268:SER:OG	2.29	0.44
2:B:424:LYS:HD2	2:B:424:LYS:HA	1.74	0.44
1:C:157:PRO:O	1:C:161:GLN:HG2	2.18	0.44
2:D:125:ARG:NE	2:D:147:ASN:HA	2.33	0.44
2:D:197:GLN:HA	2:D:197:GLN:OE1	2.18	0.44
1:A:115:TYR:CD2	4:P:822:DG:H2''	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:161:GLN:NE2	2:B:165:THR:HG23	2.33	0.44
2:B:186:ASP:OD2	2:B:409:THR:OG1	2.32	0.44
2:D:370:GLU:O	2:D:374:LYS:HG3	2.17	0.44
1:A:496:VAL:HG22	1:A:534:ALA:HB3	1.99	0.43
2:B:257:ILE:HB	2:B:283:LEU:HD21	2.00	0.43
1:C:114:ALA:HB1	1:C:160:PHE:CZ	2.53	0.43
2:B:37:ILE:O	2:B:41:MET:HG3	2.17	0.43
2:D:103:LYS:HD2	2:D:190:GLY:C	2.43	0.43
2:D:171:PHE:CD2	2:D:205:LEU:HD13	2.53	0.43
4:P:814:DC:H2''	4:P:815:DG:C8	2.54	0.43
1:C:97:PRO:HA	1:C:100:LEU:HG	2.01	0.43
2:D:27:THR:O	2:D:31:ILE:HG13	2.18	0.43
2:B:219:LYS:HD2	2:B:219:LYS:N	2.34	0.43
1:C:334:GLN:HA	1:C:334:GLN:OE1	2.19	0.43
1:A:175:ASN:HB3	1:A:178:ILE:HD12	2.00	0.43
2:B:58:THR:HG21	2:B:77:PHE:CD1	2.54	0.43
1:C:205:LEU:O	1:C:209:LEU:HD12	2.18	0.43
1:C:406:TRP:CD1	1:C:407:GLN:HG2	2.54	0.43
1:A:100:LEU:O	1:A:318:TYR:HB3	2.19	0.42
2:B:395:LYS:HG3	2:B:416:PHE:CE2	2.54	0.42
1:C:38:CYS:SG	1:C:132:ILE:HD11	2.59	0.42
2:D:102:LYS:HD3	2:D:102:LYS:HA	1.76	0.42
1:A:178:ILE:HD11	1:A:201:LYS:HG2	1.99	0.42
1:C:225:PRO:HB3	1:C:227:PHE:CE1	2.55	0.42
2:B:191:SER:OG	2:B:198:HIS:ND1	2.36	0.42
4:P:815:DG:H2'	4:P:816:DG:H8	1.85	0.42
2:D:164:MET:HE3	2:D:168:LEU:HD11	2.01	0.42
1:C:230:MET:HE1	4:F:822:DG:H1'	2.00	0.42
1:C:408:ALA:O	2:D:393:ILE:HG13	2.20	0.42
1:A:270:ILE:HD12	1:A:270:ILE:HA	1.93	0.42
2:B:13:LYS:HE3	2:B:84:THR:O	2.20	0.42
1:A:31:ILE:O	1:A:35:VAL:HG23	2.20	0.41
2:D:244:ILE:HD11	2:D:426:TRP:CZ3	2.54	0.41
2:D:105:SER:O	2:D:190:GLY:HA2	2.20	0.41
1:A:77:PHE:O	1:A:81:ASN:ND2	2.53	0.41
1:C:227:PHE:HD1	1:C:234:LEU:O	2.02	0.41
1:C:244:ILE:HD13	1:C:267:ALA:HB2	2.02	0.41
1:A:77:PHE:O	1:A:81:ASN:CG	2.63	0.41
1:A:235:HIS:HB2	1:A:238:LYS:HG2	2.01	0.41
1:A:476:LYS:NZ	8:A:706:HOH:O	2.40	0.41
1:C:547:GLN:OE1	1:C:547:GLN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:LYS:HE2	1:C:116:PHE:HB3	2.02	0.41
1:A:255:ASN:O	1:A:259:LYS:HG3	2.21	0.41
2:B:60:VAL:HG12	2:B:75:VAL:HG22	2.02	0.41
1:C:11:LYS:HD2	1:C:11:LYS:N	2.35	0.41
1:C:75:VAL:HB	1:C:77:PHE:CE2	2.55	0.41
2:D:281:LYS:HG2	2:D:284:ARG:NH2	2.36	0.41
3:T:710:DG:H2'	3:T:711:DC:C6	2.56	0.41
1:C:259:LYS:HB3	1:C:259:LYS:HE2	1.72	0.41
1:C:301:LEU:O	1:C:305:GLU:HG3	2.21	0.41
1:C:350:LYS:HE2	1:C:350:LYS:HB2	1.78	0.41
1:C:367:GLN:NE2	1:C:512:LYS:HD2	2.36	0.41
2:D:369:THR:HG22	2:D:373:GLN:HE21	1.86	0.41
3:E:708:DG:H1	4:F:820:DC:H42	1.68	0.41
1:C:469:LEU:HD11	1:C:480:GLN:HG2	2.03	0.41
1:A:130:PHE:CZ	1:A:144:TYR:HB2	2.56	0.40
2:D:184:MET:HE3	2:D:184:MET:HB3	1.82	0.40
3:E:718:DA:H2''	3:E:719:DG:C8	2.55	0.40
2:D:49:LYS:HB3	2:D:49:LYS:HE3	1.70	0.40
2:D:353:LYS:HE3	2:D:353:LYS:HB3	1.88	0.40
3:E:710:DG:H2'	3:E:711:DC:C6	2.56	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	553/556 (100%)	537 (97%)	16 (3%)	0	100	100
1	C	549/556 (99%)	531 (97%)	18 (3%)	0	100	100
2	B	413/444 (93%)	399 (97%)	14 (3%)	0	100	100
2	D	400/444 (90%)	390 (98%)	9 (2%)	1 (0%)	36	54
All	All	1915/2000 (96%)	1857 (97%)	57 (3%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	420	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	496/497 (100%)	496 (100%)	0	100	100
1	C	492/497 (99%)	485 (99%)	7 (1%)	59	78
2	B	379/403 (94%)	372 (98%)	7 (2%)	51	73
2	D	369/403 (92%)	364 (99%)	5 (1%)	59	78
All	All	1736/1800 (96%)	1717 (99%)	19 (1%)	65	81

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	5	ILE
2	B	86	ASP
2	B	179	VAL
2	B	362	THR
2	B	419	THR
2	B	423	VAL
2	B	425	LEU
1	C	92	LEU
1	C	110	ASP
1	C	245	VAL
1	C	253	THR
1	C	379	SER
1	C	428	GLN
1	C	475	GLN
2	D	163	SER
2	D	233	GLU
2	D	418	ASN
2	D	423	VAL
2	D	424	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	315	HIS
1	A	332	GLN
1	A	487	GLN
1	A	520	GLN
1	A	547	GLN
2	B	161	GLN
2	B	269	GLN
1	C	373	GLN
1	C	464	GLN
1	C	475	GLN
2	D	137	ASN
2	D	255	ASN
2	D	315	HIS
2	D	373	GLN
2	D	394	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](#)

Of 30 ligands modelled in this entry, 28 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
6	SO4	A	608	5	4,4,4	0.25	0	6,6,6	0.15	0
6	SO4	B	504	-	4,4,4	0.23	0	6,6,6	0.10	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
6	B	504	SO4	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	555/556 (99%)	0.09	13 (2%) 61 52	26, 48, 85, 125	0
1	C	551/556 (99%)	0.68	46 (8%) 17 13	29, 74, 117, 145	0
2	B	417/444 (93%)	0.11	22 (5%) 32 24	25, 46, 76, 108	0
2	D	406/444 (91%)	0.63	39 (9%) 13 11	32, 65, 111, 149	0
3	E	24/28 (85%)	0.56	3 (12%) 8 6	74, 86, 112, 139	0
3	T	25/28 (89%)	-0.12	0 100 100	35, 61, 96, 110	0
4	F	21/21 (100%)	0.19	1 (4%) 35 28	58, 87, 104, 127	0
4	P	21/21 (100%)	-0.36	0 100 100	43, 53, 82, 96	0
All	All	2020/2098 (96%)	0.36	124 (6%) 27 20	25, 57, 108, 149	0

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	88	TRP	4.8
2	B	360	ALA	4.6
2	D	5	ILE	4.6
1	A	77	PHE	4.5
2	D	214	LEU	4.3
2	D	229	TRP	4.1
2	B	423	VAL	4.0
2	B	361	HIS	4.0
2	B	357	MET	3.9
1	C	25	PRO	3.9
2	D	94	ILE	3.9
2	D	95	PRO	3.8
2	D	88	TRP	3.7
1	C	66	LYS	3.5
1	C	18	GLY	3.5
2	B	217	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
2	D	405	TYR	3.5
3	E	704	DA	3.4
2	B	218	ASP	3.4
2	D	67	ASP	3.4
2	D	66	LYS	3.3
1	C	185	ASP	3.2
1	C	33	ALA	3.2
2	D	61	PHE	3.2
2	D	90	VAL	3.1
2	D	419	THR	3.1
1	C	64	LYS	3.0
1	A	140	PRO	3.0
1	C	4	PRO	3.0
2	D	195	ILE	3.0
1	C	193	LEU	3.0
2	D	86	ASP	3.0
2	D	213	GLY	2.9
1	C	251	SER	2.9
2	B	66	LYS	2.9
1	C	144	TYR	2.9
1	C	91	GLN	2.9
2	D	357	MET	2.9
2	B	420	PRO	2.8
2	B	195	ILE	2.8
2	D	112	GLY	2.8
1	C	70	LYS	2.8
1	C	63	CYS	2.8
2	B	213	GLY	2.8
2	B	356	ARG	2.7
2	D	87	PHE	2.7
1	C	181	TYR	2.7
2	B	95	PRO	2.7
1	C	245	VAL	2.7
2	B	358	ARG	2.7
2	D	426	TRP	2.7
2	D	428	GLN	2.7
2	D	362	THR	2.6
2	D	92	LEU	2.6
2	B	5	ILE	2.6
1	C	47	ILE	2.6
2	D	233	GLU	2.6
1	C	554	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	227	PHE	2.6
3	E	725	DG	2.6
1	C	219	LYS	2.6
1	C	226	PRO	2.6
1	A	135	ILE	2.6
1	C	69	THR	2.6
2	D	116	PHE	2.6
1	A	70	LYS	2.5
2	D	210	LEU	2.5
1	C	37	ILE	2.5
1	C	292	VAL	2.5
1	C	19	PRO	2.5
2	D	24	TRP	2.5
2	B	362	THR	2.5
1	C	274	ILE	2.5
1	C	252	TRP	2.5
2	B	427	TYR	2.4
2	D	407	GLN	2.4
1	C	74	LEU	2.4
1	C	5	ILE	2.4
1	A	134	SER	2.4
1	C	171	PHE	2.4
2	D	89	GLU	2.4
2	D	421	PRO	2.4
1	A	38	CYS	2.3
2	D	71	TRP	2.3
2	B	419	THR	2.3
2	D	427	TYR	2.3
1	A	137	ASN	2.3
1	C	92	LEU	2.3
3	E	726	DT	2.3
1	C	428	GLN	2.3
2	D	180	ILE	2.2
2	D	315	HIS	2.2
1	A	139	THR	2.2
1	C	24	TRP	2.2
1	C	111	VAL	2.2
1	C	140	PRO	2.2
2	D	420	PRO	2.2
2	D	93	GLY	2.2
4	F	822	DG	2.2
1	C	286	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	232	TYR	2.2
1	C	141	GLY	2.2
1	C	137	ASN	2.2
1	C	71	TRP	2.2
1	C	302	GLU	2.2
1	C	195	ILE	2.2
1	C	386	THR	2.2
1	A	288	ALA	2.2
1	A	133	PRO	2.1
1	C	230	MET	2.1
1	C	30	LYS	2.1
2	D	318	TYR	2.1
1	C	158	ALA	2.1
2	B	425	LEU	2.1
2	D	85	GLN	2.1
1	C	294	PRO	2.1
1	C	313	PRO	2.1
1	A	15	GLY	2.1
1	A	75	VAL	2.0
2	B	226	PRO	2.0
2	B	290	THR	2.0
1	C	184	MET	2.0
2	D	425	LEU	2.0
1	A	69	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 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($\text{\AA}^2$)	Q<0.9
7	MG	C	604	1/1	0.34	0.31	90,90,90,90	0
5	CD	E	802	1/1	0.67	0.14	143,143,143,143	0
5	CD	E	803	1/1	0.89	0.10	143,143,143,143	0
5	CD	E	801	1/1	0.89	0.07	119,119,119,119	0
6	SO4	B	504	5/5	0.90	0.12	60,66,72,75	0
5	CD	C	603	1/1	0.92	0.11	99,99,99,99	0
5	CD	A	605	1/1	0.92	0.08	129,129,129,129	0
6	SO4	A	608	5/5	0.93	0.09	49,66,71,75	0
5	CD	A	607	1/1	0.93	0.06	116,116,116,116	0
5	CD	F	902	1/1	0.93	0.07	141,141,141,141	0
5	CD	F	901	1/1	0.94	0.06	133,133,133,133	0
5	CD	D	503	1/1	0.95	0.08	149,149,149,149	0
5	CD	T	804	1/1	0.96	0.05	123,123,123,123	0
5	CD	P	902	1/1	0.96	0.07	112,112,112,112	0
5	CD	A	604	1/1	0.96	0.06	97,97,97,97	0
5	CD	T	802	1/1	0.96	0.04	125,125,125,125	0
5	CD	B	502	1/1	0.97	0.04	89,89,89,89	0
5	CD	T	803	1/1	0.97	0.04	112,112,112,112	0
5	CD	A	606	1/1	0.98	0.04	72,72,72,72	0
5	CD	A	601	1/1	0.98	0.04	48,48,48,48	0
5	CD	B	501	1/1	0.98	0.04	66,66,66,66	0
5	CD	D	501	1/1	0.99	0.03	78,78,78,78	0
5	CD	P	901	1/1	0.99	0.02	83,83,83,83	0
5	CD	T	801	1/1	0.99	0.03	70,70,70,70	0
5	CD	C	602	1/1	0.99	0.06	62,62,62,62	0
5	CD	A	602	1/1	0.99	0.09	66,66,66,66	0
5	CD	B	503	1/1	1.00	0.01	57,57,57,57	0
5	CD	C	601	1/1	1.00	0.04	48,48,48,48	0
5	CD	D	502	1/1	1.00	0.03	58,58,58,58	0
5	CD	A	603	1/1	1.00	0.02	60,60,60,60	0

6.5 Other polymers

There are no such residues in this entry.