



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2016 – 04:43 PM EDT

PDB ID : 5HRO
Title : STRUCTURE OF HIV-1 REVERSE TRANSCRIPTASE In COMPLEX
WITH A DNA aptamer and an Alpha-carboxy nucleoside phosphonate in-
hibitor (alpha-CNP)
Authors : Das, K.; Arnold, E.
Deposited on : 2016-01-23
Resolution : 2.75 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
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) : rb-20027939

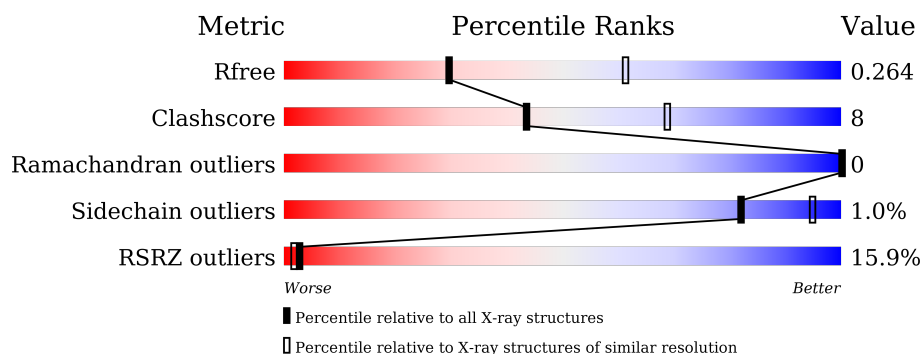
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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 ≥ 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	555	<div> <div>17%</div> <div> <div></div> <div>76%</div> <div>23%</div> <div>.</div> </div> </div>
1	C	555	<div> <div>24%</div> <div> <div></div> <div>75%</div> <div>24%</div> <div>..</div> </div> </div>
2	B	444	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>14%</div> <div>7%</div> </div> </div>
2	D	444	<div> <div>12%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>7%</div> </div> </div>
3	E	38	<div> <div></div> <div> <div></div> <div>61%</div> <div>32%</div> <div>8%</div> </div> </div>
3	F	38	<div> <div>5%</div> <div> <div></div> <div>55%</div> <div>34%</div> <div>.</div> <div>8%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SO4	B	504	-	-	-	X
6	SO4	B	505	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 17349 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 HIV-1 REVERSE TRANSCRIPTASE P66 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	0	0
			4488	2905	747	829	7			
1	C	551	Total	C	N	O	S	0	0	0
			4488	2905	747	829	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	SER	CYS	engineered mutation	UNP P03366
C	280	SER	CYS	engineered mutation	UNP P03366

- Molecule 2 is a protein called HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	412	Total	C	N	O	S	0	0	0
			3400	2212	563	619	6			
2	D	412	Total	C	N	O	S	0	0	0
			3400	2212	563	619	6			

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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 (38-MER).

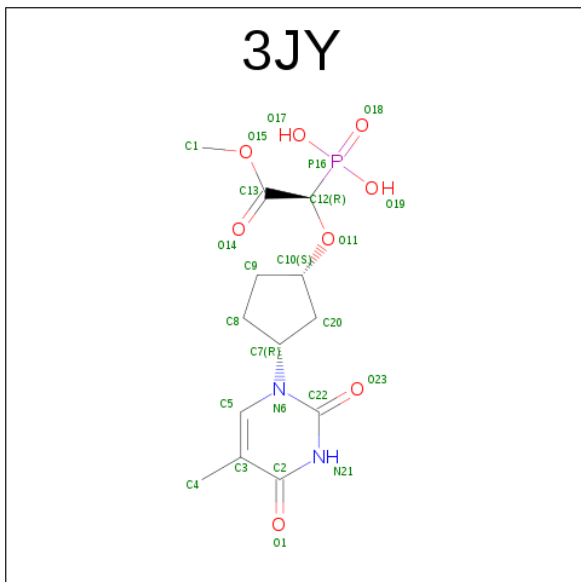
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	35	Total	C	N	O	P	0	0	0
			720	340	130	215	35			
3	F	35	Total	C	N	O	P	0	0	0
			720	340	130	215	35			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Mg	0	0
			3	3		
4	C	3	Total	Mg	0	0
			3	3		

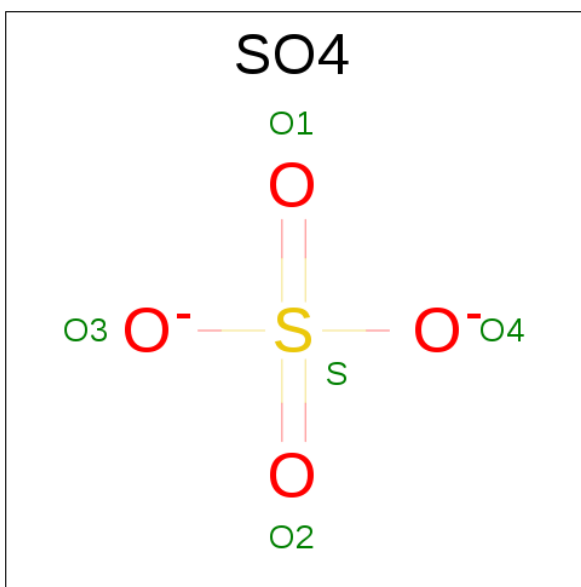
- Molecule 5 is [(1R)-2-methoxy-1-[(1S,3R)-3-(5-methyl-2,4-dioxo-3,4-dihydropyrimidin

-1(2H)-yl)cyclopentyl]oxy}-2-oxoethyl]phosphonic acid (three-letter code: 3JY) (formula: $C_{13}H_{19}N_2O_8P$).



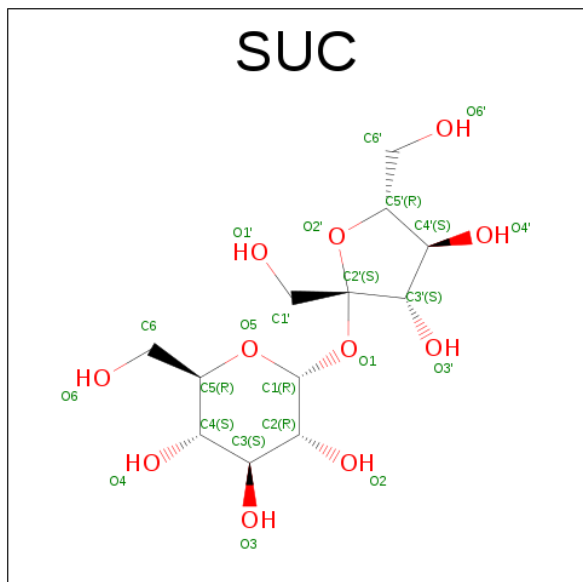
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			23	12	2	8	1		
5	C	1	Total	C	N	O	P	0	0
			23	12	2	8	1		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 7 is SUCROSE (three-letter code: SUC) (formula: $C_{12}H_{22}O_{11}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 23 12 11	0	0
7	D	1	Total C O 23 12 11	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O 1 1	0	0
8	B	1	Total O 1 1	0	0

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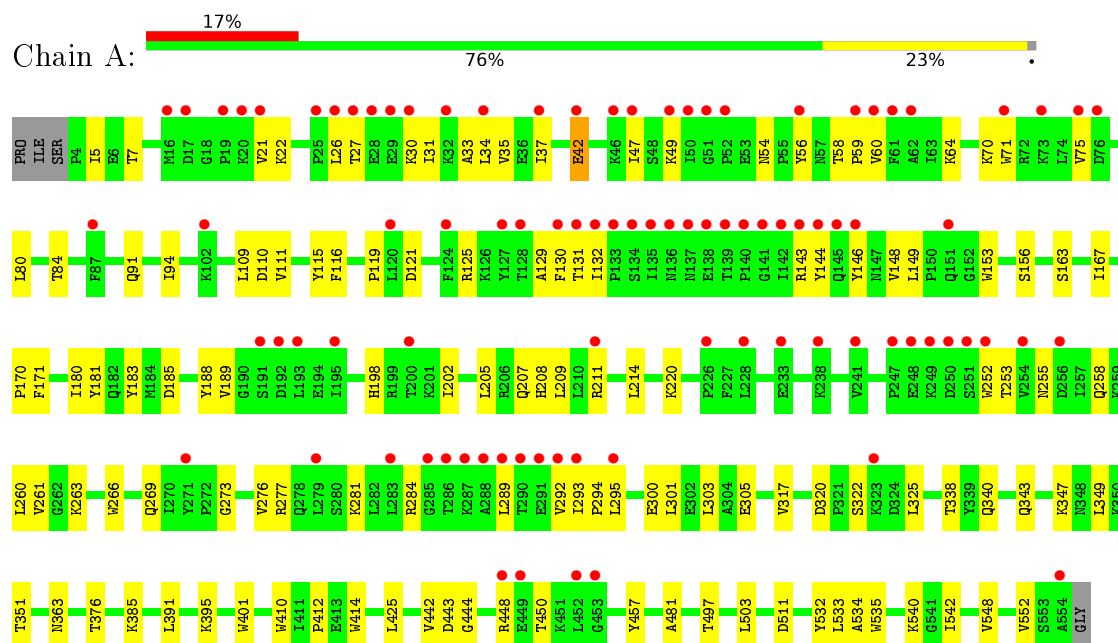
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	3	Total	O	0	0
			3	3		

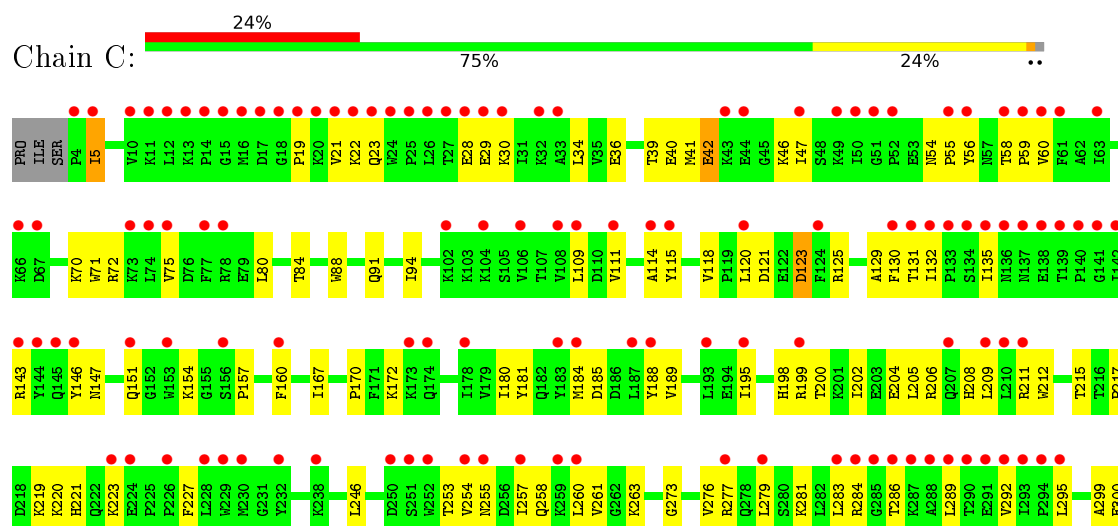
3 Residue-property plots

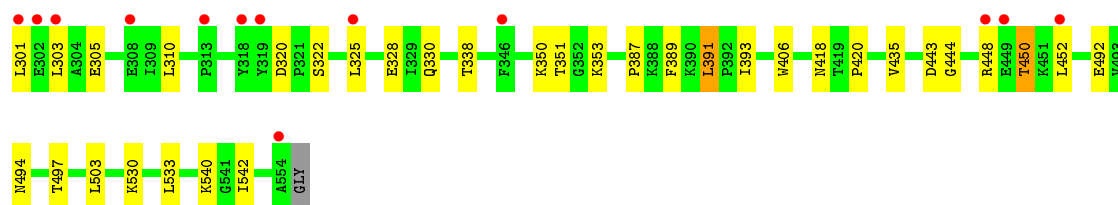
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: HIV-1 REVERSE TRANSCRIPTASE P66 SUBUNIT

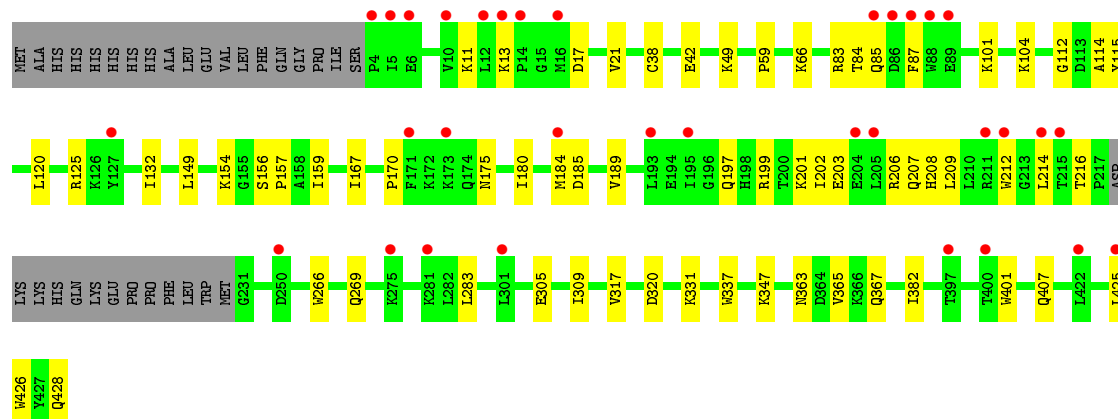
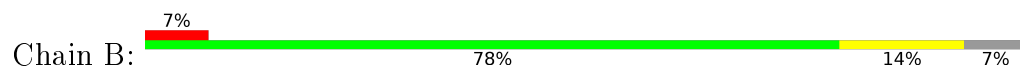


• Molecule 1: HIV-1 REVERSE TRANSCRIPTASE P66 SUBUNIT

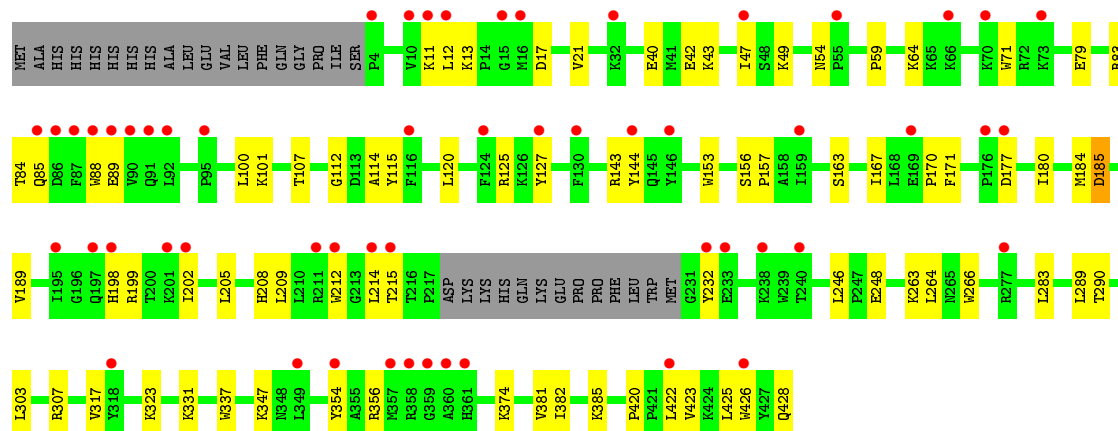
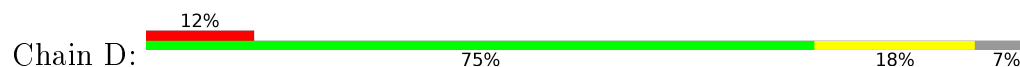




• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT



• Molecule 2: HIV-1 REVERSE TRANSCRIPTASE P51 SUBUNIT



• Molecule 3: DNA (38-MER)



• Molecule 3: DNA (38-MER)





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.25Å 128.96Å 131.05Å 90.00° 101.47° 90.00°	Depositor
Resolution (Å)	38.52 – 2.75 38.52 – 2.73	Depositor EDS
% Data completeness (in resolution range)	95.8 (38.52-2.75) 94.7 (38.52-2.73)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.72Å)	Xtriage
Refinement program	PHENIX (1.10 _2155: ???)	Depositor
R, R_{free}	0.235 , 0.265 0.234 , 0.264	Depositor DCC
R_{free} test set	2911 reflections (3.98%)	DCC
Wilson B-factor (Å ²)	73.1	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 62.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17349	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: OMC, MG, 3JY, SUC, SO4

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	0.28	0/4605	0.49	0/6255
1	C	0.28	0/4605	0.49	1/6255 (0.0%)
2	B	0.27	0/3497	0.47	0/4751
2	D	0.29	0/3497	0.49	0/4751
3	E	0.64	1/759 (0.1%)	1.01	0/1170
3	F	0.72	3/759 (0.4%)	1.01	2/1170 (0.2%)
All	All	0.33	4/17722 (0.0%)	0.56	3/24352 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	26	DC	C4'-O4'	7.28	1.52	1.45
3	F	19	DC	C4'-O4'	5.75	1.50	1.45
3	E	24	DC	C4'-O4'	5.24	1.50	1.45
3	F	24	DC	C4'-O4'	5.10	1.50	1.45

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	7	DC	O4'-C4'-C3'	-6.52	101.89	104.50
3	F	19	DC	O4'-C4'-C3'	-6.06	102.08	104.50
1	C	55	PRO	N-CA-C	5.21	125.65	112.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4488	0	4545	86	0
1	C	4488	0	4545	95	0
2	B	3400	0	3431	41	0
2	D	3400	0	3430	54	0
3	E	720	0	396	13	0
3	F	720	0	396	12	0
4	A	3	0	0	0	0
4	C	3	0	0	0	0
5	A	23	0	14	0	0
5	C	23	0	14	4	0
6	A	5	0	0	0	0
6	B	20	0	0	0	0
6	C	5	0	0	0	0
7	B	23	0	22	0	0
7	D	23	0	22	1	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	3	0	0	0	0
All	All	17349	0	16815	278	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 8.

All (278) 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:A:255:ASN:HB2	1:A:289:LEU:HD21	1.27	1.09
1:A:255:ASN:HB2	1:A:289:LEU:CD2	1.98	0.92
1:C:221:HIS:HE1	1:C:223:LYS:HG3	1.39	0.88
1:A:255:ASN:CB	1:A:289:LEU:HD21	2.11	0.80
1:C:255:ASN:HB2	1:C:289:LEU:CD2	2.10	0.80
2:D:248:GLU:OE1	2:D:307:ARG:NH2	2.15	0.80
1:C:56:TYR:HB2	1:C:129:ALA:HB3	1.65	0.78
1:C:221:HIS:CE1	1:C:223:LYS:HG3	2.20	0.76
1:A:110:ASP:HB3	1:A:220:LYS:HB3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:ASN:HB2	1:C:289:LEU:HD21	1.71	0.71
5:C:605:3JY:H11	5:C:605:3JY:H6	1.73	0.70
1:C:261:VAL:HG13	1:C:276:VAL:HG11	1.72	0.70
1:C:172:LYS:HE2	1:C:180:ILE:HB	1.75	0.69
1:A:56:TYR:HB2	1:A:129:ALA:HB3	1.74	0.69
2:D:115:TYR:CD2	2:D:156:SER:HB3	2.28	0.69
1:C:72:ARG:NH1	5:C:605:3JY:O19	2.26	0.68
1:C:111:VAL:HB	1:C:185:ASP:HB2	1.75	0.67
1:A:207:GLN:O	1:A:211:ARG:N	2.26	0.67
1:A:261:VAL:HG13	1:A:276:VAL:HG11	1.76	0.66
2:D:180:ILE:HG12	2:D:189:VAL:HG22	1.78	0.66
1:A:255:ASN:HD22	1:A:289:LEU:HD11	1.62	0.63
1:A:183:TYR:OH	3:E:36:DG:N3	2.29	0.63
1:C:60:VAL:HG22	1:C:75:VAL:HG13	1.79	0.63
1:C:41:MET:HB3	1:C:46:LYS:HB2	1.81	0.62
1:C:19:PRO:HB2	1:C:58:THR:HG23	1.79	0.62
1:A:94:ILE:HD11	3:E:35:DG:H21	1.65	0.62
3:E:27:DC:H2"	3:E:28:DG:C8	2.35	0.61
1:C:5:ILE:HG22	1:C:212:TRP:HD1	1.64	0.61
2:B:206:ARG:NH2	2:B:216:THR:O	2.33	0.61
2:B:13:LYS:HD2	2:B:85:GLN:HB3	1.83	0.61
1:A:64:LYS:HA	1:A:71:TRP:HA	1.83	0.61
1:A:21:VAL:HG23	1:A:59:PRO:HD3	1.82	0.60
1:A:448:ARG:HH21	3:E:22:DT:H5"	1.65	0.60
2:D:199:ARG:HA	2:D:202:ILE:HD12	1.84	0.60
1:C:184:MET:HG2	3:F:37:DG:H2"	1.83	0.59
2:B:180:ILE:HG12	2:B:189:VAL:HG22	1.84	0.59
1:A:253:THR:HA	1:A:292:VAL:HA	1.85	0.59
1:C:118:VAL:HG21	1:C:160:PHE:HD1	1.68	0.59
2:D:246:LEU:HD11	2:D:264:LEU:HD21	1.84	0.59
2:D:266:TRP:NE1	2:D:425:LEU:HD22	2.17	0.59
2:D:170:PRO:HB2	2:D:208:HIS:CE1	2.37	0.58
1:C:257:ILE:HB	1:C:283:LEU:HD21	1.85	0.58
2:B:157:PRO:HG3	2:B:184:MET:HA	1.85	0.58
2:B:115:TYR:CD2	2:B:156:SER:HB3	2.38	0.58
1:A:70:LYS:HG2	1:A:71:TRP:H	1.69	0.58
1:A:209:LEU:HB3	1:A:214:LEU:HB2	1.86	0.57
1:A:542:ILE:HG23	2:B:283:LEU:HD13	1.87	0.57
1:C:180:ILE:HG23	1:C:189:VAL:HG22	1.87	0.57
1:C:125:ARG:HE	1:C:147:ASN:HA	1.68	0.57
2:B:170:PRO:HB2	2:B:208:HIS:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:ILE:O	1:C:206:ARG:HG3	2.06	0.56
2:D:21:VAL:HB	2:D:59:PRO:HD3	1.87	0.56
2:D:114:ALA:HB2	2:D:214:LEU:HD22	1.88	0.56
2:B:199:ARG:HA	2:B:202:ILE:HD12	1.87	0.56
1:C:23:GLN:NE2	1:C:131:THR:O	2.38	0.56
1:C:219:LYS:HE2	1:C:220:LYS:HE2	1.88	0.56
1:C:5:ILE:HG22	1:C:212:TRP:CD1	2.40	0.55
1:C:23:GLN:HG3	1:C:131:THR:HG23	1.89	0.55
1:C:181:TYR:HB2	1:C:188:TYR:HB3	1.87	0.55
2:D:198:HIS:CD2	2:D:202:ILE:HD11	2.42	0.55
1:C:279:LEU:HD23	1:C:299:ALA:HB1	1.88	0.55
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.89	0.54
1:A:34:LEU:HD21	1:A:132:ILE:HD12	1.88	0.54
2:B:114:ALA:HB2	2:B:214:LEU:HD22	1.88	0.54
1:C:123:ASP:N	1:C:123:ASP:OD1	2.40	0.54
3:E:12:DT:H2'	3:E:13:DT:H71	1.89	0.54
1:A:395:LYS:NZ	1:A:414:TRP:O	2.40	0.54
2:B:363:ASN:O	2:B:367:GLN:HG3	2.08	0.54
2:B:17:ASP:O	2:B:83:ARG:NH1	2.40	0.54
1:C:253:THR:HA	1:C:292:VAL:HA	1.90	0.54
1:A:252:TRP:O	1:A:292:VAL:HG23	2.09	0.53
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.91	0.53
2:B:331:LYS:HB2	2:B:337:TRP:CZ3	2.43	0.53
1:C:72:ARG:NH2	5:C:605:3JY:O19	2.42	0.53
1:C:255:ASN:HB2	1:C:289:LEU:HD23	1.89	0.53
1:C:258:GLN:CD	3:F:32:DG:H2''	2.28	0.53
1:A:281:LYS:O	1:A:284:ARG:HG2	2.07	0.53
1:C:281:LYS:O	1:C:284:ARG:HG2	2.09	0.53
2:B:87:PHE:HZ	2:B:159:ILE:HG13	1.73	0.53
1:C:60:VAL:HG21	1:C:130:PHE:CD2	2.44	0.53
1:A:180:ILE:HG23	1:A:189:VAL:HG22	1.89	0.53
1:C:255:ASN:CB	1:C:289:LEU:HD21	2.38	0.53
2:D:54:ASN:HB3	2:D:143:ARG:HH21	1.74	0.52
1:C:202:ILE:HG22	1:C:206:ARG:HD2	1.90	0.52
2:B:167:ILE:HG23	2:B:212:TRP:CD1	2.44	0.52
2:D:64:LYS:HE3	2:D:71:TRP:CE2	2.45	0.52
1:A:273:GLY:HA2	1:A:338:THR:HG21	1.91	0.52
1:A:94:ILE:HD11	3:E:35:DG:N2	2.25	0.52
1:C:448:ARG:HH21	3:F:22:DT:H5''	1.73	0.52
1:A:503:LEU:HD22	1:A:535:TRP:HB2	1.90	0.52
2:B:203:GLU:O	2:B:207:GLN:HG2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:ILE:HD12	3:F:8:OMC:HM23	1.91	0.51
2:D:263:LYS:HA	2:D:423:VAL:HG21	1.92	0.51
2:B:365:VAL:HG11	2:B:401:TRP:HB2	1.93	0.51
1:A:27:THR:O	1:A:31:ILE:HG13	2.10	0.51
1:A:111:VAL:HB	1:A:185:ASP:HB2	1.93	0.51
2:D:115:TYR:HD2	2:D:156:SER:HB3	1.75	0.51
2:D:266:TRP:CD1	2:D:425:LEU:HD13	2.46	0.51
2:D:13:LYS:HD2	2:D:85:GLN:HB3	1.93	0.51
1:A:47:ILE:HG13	1:A:144:TYR:HB3	1.94	0.50
1:A:260:LEU:HD21	1:A:303:LEU:HD13	1.93	0.50
1:A:503:LEU:HD11	1:A:533:LEU:HB3	1.92	0.50
2:B:197:GLN:O	2:B:201:LYS:HG2	2.12	0.50
2:D:84:THR:HG21	2:D:153:TRP:HZ2	1.77	0.50
2:D:425:LEU:HD23	2:D:426:TRP:CE2	2.47	0.50
3:E:7:DC:H2'	3:E:8:OMC:C6	2.47	0.50
3:E:7:DC:H2'	3:E:8:OMC:H6	1.77	0.49
1:C:492:GLU:HG2	1:C:530:LYS:HB2	1.94	0.49
2:B:167:ILE:HG12	2:B:212:TRP:CD2	2.47	0.49
2:B:209:LEU:HD13	2:B:214:LEU:HD23	1.94	0.49
2:D:209:LEU:HD13	2:D:214:LEU:HD23	1.94	0.49
1:A:293:ILE:HG13	1:A:294:PRO:HD2	1.95	0.49
1:C:260:LEU:HD21	1:C:303:LEU:HD13	1.94	0.49
1:A:47:ILE:HD12	1:A:146:TYR:HA	1.95	0.49
2:B:320:ASP:OD2	1:C:418:ASN:ND2	2.39	0.49
2:D:42:GLU:OE2	2:D:49:LYS:HG3	2.12	0.49
2:B:21:VAL:HB	2:B:59:PRO:HD3	1.94	0.48
1:C:28:GLU:HB2	1:C:135:ILE:HD12	1.95	0.48
2:D:120:LEU:HD23	2:D:125:ARG:HG2	1.94	0.48
1:A:443:ASP:OD1	1:A:444:GLY:N	2.46	0.48
2:D:177:ASP:N	2:D:177:ASP:OD1	2.37	0.48
2:D:356:ARG:HG3	2:D:356:ARG:O	2.13	0.48
1:A:548:VAL:O	1:A:552:VAL:HG22	2.14	0.48
3:F:17:DT:H4'	3:F:18:DG:OP1	2.14	0.48
1:C:542:ILE:HG23	2:D:283:LEU:HD13	1.94	0.48
1:C:205:LEU:O	1:C:209:LEU:HG	2.14	0.48
2:D:167:ILE:HG23	2:D:212:TRP:CD1	2.49	0.48
1:A:110:ASP:HB3	1:A:220:LYS:CB	2.43	0.47
1:C:70:LYS:HG2	1:C:71:TRP:H	1.79	0.47
1:A:301:LEU:O	1:A:305:GLU:HG2	2.14	0.47
1:A:5:ILE:HD11	1:A:163:SER:HB3	1.96	0.47
2:B:317:VAL:HG12	2:B:347:LYS:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:ASN:ND2	1:C:289:LEU:HD21	2.29	0.47
2:D:17:ASP:O	2:D:83:ARG:HD3	2.14	0.47
1:A:30:LYS:HG2	1:A:71:TRP:CZ3	2.50	0.47
1:C:254:VAL:HG13	1:C:283:LEU:HD22	1.94	0.47
1:C:391:LEU:HB3	1:C:393:ILE:HG22	1.97	0.47
2:D:428:GLN:HA	2:D:428:GLN:HE21	1.80	0.47
1:C:389:PHE:HB3	1:C:391:LEU:HD13	1.97	0.47
1:C:540:LYS:HA	1:C:540:LYS:HD3	1.68	0.47
2:D:100:LEU:HG	2:D:381:VAL:HG13	1.96	0.47
1:A:317:VAL:HG11	1:A:347:LYS:HB3	1.97	0.47
2:D:163:SER:O	2:D:167:ILE:HG13	2.15	0.47
1:C:494:ASN:HB3	2:D:289:LEU:HD12	1.96	0.47
1:A:167:ILE:O	1:A:170:PRO:HD2	2.14	0.47
1:C:263:LYS:HD2	3:F:34:DG:H4'	1.97	0.47
1:A:266:TRP:O	1:A:269:GLN:HG2	2.15	0.47
1:C:114:ALA:HB1	1:C:160:PHE:CE1	2.50	0.47
5:C:605:3JY:H3	5:C:605:3JY:H6	1.58	0.47
1:C:120:LEU:HD12	1:C:121:ASP:H	1.80	0.46
2:D:266:TRP:CD1	2:D:266:TRP:C	2.89	0.46
2:D:112:GLY:HA2	2:D:115:TYR:CD1	2.51	0.46
2:D:79:GLU:HG3	2:D:83:ARG:HE	1.80	0.46
3:F:17:DT:H2''	3:F:18:DG:C8	2.50	0.46
1:A:31:ILE:O	1:A:35:VAL:HG23	2.14	0.46
2:B:115:TYR:O	2:B:149:LEU:HB2	2.16	0.46
1:A:263:LYS:HD2	3:E:34:DG:H4'	1.97	0.46
1:A:121:ASP:O	1:A:125:ARG:HG3	2.15	0.46
2:B:66:LYS:NZ	2:B:407:GLN:OE1	2.39	0.46
1:C:125:ARG:NE	1:C:147:ASN:HA	2.30	0.46
1:C:131:THR:HB	1:C:143:ARG:HG2	1.98	0.46
1:C:29:GLU:HG3	1:C:30:LYS:N	2.31	0.46
1:C:167:ILE:O	1:C:170:PRO:HD2	2.16	0.46
1:C:200:THR:O	1:C:204:GLU:HG3	2.16	0.46
1:A:376:THR:HG21	2:B:401:TRP:CH2	2.51	0.46
1:C:198:HIS:O	1:C:202:ILE:HG12	2.16	0.46
2:B:428:GLN:HA	2:B:428:GLN:HE21	1.80	0.45
1:C:34:LEU:HD21	1:C:132:ILE:HD12	1.98	0.45
2:D:12:LEU:HD11	2:D:127:TYR:CE1	2.50	0.45
1:A:7:THR:OG1	1:A:121:ASP:HA	2.16	0.45
1:A:60:VAL:HG22	1:A:75:VAL:HG13	1.98	0.45
2:B:38:CYS:SG	2:B:132:ILE:HD11	2.56	0.45
1:C:273:GLY:HA2	1:C:338:THR:HG21	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ASN:O	1:A:143:ARG:NH2	2.49	0.45
2:B:154:LYS:HG2	2:B:184:MET:SD	2.57	0.45
1:A:5:ILE:HD12	1:A:167:ILE:HD11	1.99	0.45
1:A:340:GLN:HG3	1:A:351:THR:HG22	1.98	0.45
1:C:211:ARG:HB2	1:C:212:TRP:CE3	2.52	0.45
1:C:184:MET:HE3	1:C:184:MET:HA	1.97	0.45
1:C:227:PHE:N	1:C:227:PHE:CD2	2.84	0.45
2:D:171:PHE:CD2	2:D:205:LEU:HD13	2.51	0.45
1:C:80:LEU:O	1:C:84:THR:OG1	2.33	0.45
1:A:116:PHE:O	1:A:148:VAL:HG11	2.17	0.45
1:A:295:LEU:HB3	1:A:300:GLU:HG2	1.99	0.45
2:D:40:GLU:HA	2:D:43:LYS:HG2	1.98	0.45
1:A:395:LYS:HD2	1:A:414:TRP:CH2	2.52	0.44
1:C:246:LEU:HD11	1:C:310:LEU:HD22	1.99	0.44
1:C:320:ASP:OD1	1:C:322:SER:OG	2.29	0.44
1:A:153:TRP:HB3	1:A:156:SER:OG	2.17	0.44
2:D:88:TRP:CE3	2:D:89:GLU:HG3	2.52	0.44
1:C:54:ASN:O	1:C:143:ARG:NH2	2.50	0.44
2:B:112:GLY:HA2	2:B:115:TYR:CD1	2.53	0.44
1:C:338:THR:HG22	1:C:353:LYS:HB3	2.00	0.44
2:D:303:LEU:HG	2:D:307:ARG:NH1	2.33	0.44
2:D:331:LYS:HB2	2:D:337:TRP:CZ3	2.53	0.44
7:D:501:SUC:H1	7:D:501:SUC:H1'2	1.35	0.44
1:A:171:PHE:CD2	1:A:205:LEU:HD13	2.53	0.44
1:C:258:GLN:NE2	3:F:32:DG:H2''	2.33	0.44
1:C:36:GLU:O	1:C:40:GLU:HG3	2.18	0.44
1:A:60:VAL:HG21	1:A:130:PHE:CD2	2.53	0.44
2:B:425:LEU:HD23	2:B:426:TRP:CE2	2.52	0.43
1:C:21:VAL:HG23	1:C:59:PRO:HD3	2.00	0.43
2:D:317:VAL:HG12	2:D:347:LYS:HB3	1.98	0.43
1:A:325:LEU:HD12	1:A:385:LYS:HG3	2.00	0.43
2:B:101:LYS:HD3	2:B:382:ILE:HG23	2.01	0.43
2:D:323:LYS:O	2:D:385:LYS:NZ	2.50	0.43
1:A:320:ASP:OD1	1:A:322:SER:OG	2.25	0.43
1:C:418:ASN:O	1:C:420:PRO:HD3	2.18	0.43
1:A:532:TYR:CE2	1:A:534:ALA:HB2	2.53	0.43
2:D:47:ILE:HD12	2:D:144:TYR:CD2	2.53	0.43
1:C:435:VAL:HG22	2:D:290:THR:HG21	2.00	0.43
1:A:70:LYS:HG2	1:A:71:TRP:N	2.32	0.43
1:C:91:GLN:O	3:F:7:DC:H4'	2.19	0.43
1:C:157:PRO:HG2	3:F:6:OMC:H1'	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:HIS:O	1:A:211:ARG:HB2	2.19	0.43
2:D:354:TYR:HD2	2:D:374:LYS:HD3	1.83	0.43
1:C:115:TYR:CD2	1:C:151:GLN:HG2	2.53	0.43
1:C:443:ASP:OD1	1:C:444:GLY:N	2.47	0.43
2:B:305:GLU:O	2:B:309:ILE:HG13	2.19	0.42
1:C:295:LEU:HB3	1:C:300:GLU:HG2	2.00	0.42
2:D:101:LYS:HD3	2:D:382:ILE:HG23	2.01	0.42
1:A:198:HIS:O	1:A:202:ILE:HG12	2.19	0.42
1:C:88:TRP:CD1	2:D:143:ARG:NH1	2.88	0.42
2:D:107:THR:HA	2:D:232:TYR:O	2.20	0.42
1:A:442:VAL:HG12	1:A:457:TYR:HB3	2.01	0.42
1:C:450:THR:HG22	1:C:452:LEU:HG	2.00	0.42
2:D:112:GLY:HA2	2:D:115:TYR:CE1	2.55	0.42
2:D:422:LEU:HG	2:D:423:VAL:HG12	2.00	0.42
3:F:8:OMC:HM23	3:F:8:OMC:H1'	1.83	0.42
1:A:115:TYR:HB3	1:A:149:LEU:O	2.18	0.42
2:D:185:ASP:OD1	2:D:185:ASP:N	2.50	0.42
1:C:254:VAL:HG21	1:C:286:THR:HG21	2.02	0.42
1:C:39:THR:O	1:C:42:GLU:HG3	2.20	0.42
1:A:457:TYR:HA	1:A:548:VAL:HG21	2.02	0.42
2:B:120:LEU:HD23	2:B:125:ARG:HG2	2.02	0.42
1:C:84:THR:HB	1:C:154:LYS:HE2	2.02	0.42
1:A:410:TRP:CH2	1:A:412:PRO:HA	2.55	0.42
2:B:115:TYR:HE2	2:B:157:PRO:HA	1.85	0.42
1:A:91:GLN:O	3:E:7:DC:H4'	2.19	0.42
1:A:258:GLN:HB3	3:E:33:DG:H4'	2.02	0.42
1:A:22:LYS:HD3	1:A:22:LYS:HA	1.79	0.41
1:A:33:ALA:O	1:A:37:ILE:HG12	2.21	0.41
1:A:266:TRP:CE2	3:E:35:DG:H4'	2.55	0.41
1:A:5:ILE:CG2	1:A:119:PRO:HD2	2.50	0.41
2:B:104:LYS:HE2	2:B:104:LYS:HB3	1.77	0.41
2:B:42:GLU:OE2	2:B:49:LYS:HG3	2.20	0.41
3:F:27:DC:H2''	3:F:28:DG:C8	2.54	0.41
1:A:26:LEU:HD21	1:A:34:LEU:HD13	2.01	0.41
1:A:412:PRO:HD3	2:B:401:TRP:CZ2	2.55	0.41
1:C:22:LYS:HA	1:C:22:LYS:HD3	1.88	0.41
1:A:21:VAL:HG23	1:A:58:THR:HA	2.02	0.41
1:C:47:ILE:HD12	1:C:146:TYR:HA	2.02	0.41
2:D:157:PRO:HG3	2:D:184:MET:HA	2.03	0.41
2:B:185:ASP:N	2:B:185:ASP:OD1	2.54	0.41
1:A:94:ILE:CD1	3:E:35:DG:H21	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:GLN:HG3	1:A:349:LEU:HD11	2.01	0.41
1:A:5:ILE:CD1	1:A:163:SER:HB3	2.51	0.41
1:A:401:TRP:HB2	1:A:425:LEU:HD11	2.02	0.41
2:B:84:THR:HG22	2:B:87:PHE:HB3	2.03	0.41
1:C:325:LEU:HB3	1:C:387:PRO:HB3	2.03	0.41
1:C:195:ILE:O	1:C:199:ARG:HG3	2.20	0.41
2:D:422:LEU:HG	2:D:423:VAL:N	2.36	0.41
2:B:266:TRP:O	2:B:269:GLN:HG3	2.21	0.40
1:C:28:GLU:CB	1:C:135:ILE:HD12	2.51	0.40
1:C:350:LYS:NZ	1:C:351:THR:O	2.48	0.40
1:C:406:TRP:CZ2	2:D:420:PRO:HG3	2.57	0.40
2:D:214:LEU:HD12	2:D:215:THR:H	1.87	0.40
1:A:80:LEU:O	1:A:84:THR:OG1	2.32	0.40
1:A:131:THR:HB	1:A:143:ARG:HG2	2.03	0.40
2:B:175:ASN:OD1	2:B:201:LYS:HE2	2.22	0.40
1:C:255:ASN:CG	1:C:289:LEU:HD21	2.42	0.40
1:C:301:LEU:O	1:C:305:GLU:HG2	2.20	0.40
1:C:503:LEU:HD11	1:C:533:LEU:HB3	2.02	0.40
1:A:42:GLU:OE1	1:A:49:LYS:HE3	2.22	0.40
1:A:363:ASN:HA	1:A:511:ASP:OD1	2.22	0.40
1:A:540:LYS:HA	1:A:540:LYS:HD3	1.88	0.40
1:C:215:THR:O	1:C:217:PRO:HD3	2.22	0.40
1:C:328:GLU:HG2	1:C:330:GLN:NE2	2.36	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	549/555 (99%)	536 (98%)	13 (2%)	0	100	100
1	C	549/555 (99%)	533 (97%)	16 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	408/444 (92%)	396 (97%)	12 (3%)	0	100	100
2	D	408/444 (92%)	396 (97%)	12 (3%)	0	100	100
All	All	1914/1998 (96%)	1861 (97%)	53 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	492/495 (99%)	486 (99%)	6 (1%)	78	94
1	C	492/495 (99%)	483 (98%)	9 (2%)	66	90
2	B	374/403 (93%)	373 (100%)	1 (0%)	94	98
2	D	374/403 (93%)	372 (100%)	2 (0%)	92	97
All	All	1732/1796 (96%)	1714 (99%)	18 (1%)	82	95

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	GLU
1	A	109	LEU
1	A	277	ARG
1	A	391	LEU
1	A	450	THR
1	A	497	THR
2	B	11	LYS
1	C	5	ILE
1	C	42	GLU
1	C	109	LEU
1	C	123	ASP
1	C	208	HIS
1	C	277	ARG
1	C	391	LEU

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Mol	Chain	Res	Type
1	C	450	THR
1	C	497	THR
2	D	11	LYS
2	D	185	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	373	GLN
2	B	428	GLN
1	C	221	HIS
1	C	255	ASN
1	C	487	GLN
1	C	507	GLN
2	D	208	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	OMC	E	6	3	15,22,23	0.90	1 (6%)	20,31,34	1.40	1 (5%)
3	OMC	E	8	3,2	15,22,23	0.87	1 (6%)	20,31,34	1.32	2 (10%)
3	OMC	F	6	3	15,22,23	0.91	1 (6%)	20,31,34	1.35	2 (10%)
3	OMC	F	8	3,2	15,22,23	0.88	1 (6%)	20,31,34	1.46	2 (10%)

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	OMC	E	6	3	-	0/5/27/28	0/2/2/2
3	OMC	E	8	3,2	-	0/5/27/28	0/2/2/2
3	OMC	F	6	3	-	0/5/27/28	0/2/2/2
3	OMC	F	8	3,2	-	0/5/27/28	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	8	OMC	C4-N4	2.78	1.43	1.35
3	F	6	OMC	C4-N4	2.80	1.43	1.35
3	E	6	OMC	C4-N4	2.81	1.43	1.35
3	E	8	OMC	C4-N4	2.83	1.43	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	8	OMC	N4-C4-N3	2.04	120.07	116.50
3	E	8	OMC	N4-C4-N3	2.11	120.19	116.50
3	F	6	OMC	N4-C4-N3	2.12	120.21	116.50
3	F	6	OMC	C6-C5-C4	4.54	119.22	117.44
3	E	8	OMC	C6-C5-C4	4.82	119.32	117.44
3	E	6	OMC	C6-C5-C4	5.14	119.45	117.44
3	F	8	OMC	C6-C5-C4	5.41	119.55	117.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	8	OMC	2	0
3	F	6	OMC	1	0
3	F	8	OMC	2	0

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 6 are monoatomic - leaving 10 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$
5	3JY	A	603	4	15,24,25	2.43	4 (26%)	14,36,37	3.10	5 (35%)
6	SO4	A	605	-	4,4,4	0.16	0	6,6,6	0.08	0
7	SUC	B	501	-	24,24,24	0.43	0	36,36,36	0.79	1 (2%)
6	SO4	B	502	-	4,4,4	0.28	0	6,6,6	0.23	0
6	SO4	B	503	-	4,4,4	0.16	0	6,6,6	0.12	0
6	SO4	B	504	-	4,4,4	0.13	0	6,6,6	0.13	0
6	SO4	B	505	-	4,4,4	0.11	0	6,6,6	0.21	0
6	SO4	C	604	-	4,4,4	0.22	0	6,6,6	0.17	0
5	3JY	C	605	4	15,24,25	2.51	5 (33%)	14,36,37	3.10	5 (35%)
7	SUC	D	501	-	24,24,24	0.46	0	36,36,36	1.00	2 (5%)

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
5	3JY	A	603	4	-	0/4/27/29	0/2/2/2
6	SO4	A	605	-	-	0/0/0/0	0/0/0/0
7	SUC	B	501	-	-	0/12/51/51	0/2/2/2
6	SO4	B	502	-	-	0/0/0/0	0/0/0/0
6	SO4	B	503	-	-	0/0/0/0	0/0/0/0
6	SO4	B	504	-	-	0/0/0/0	0/0/0/0
6	SO4	B	505	-	-	0/0/0/0	0/0/0/0
6	SO4	C	604	-	-	0/0/0/0	0/0/0/0
5	3JY	C	605	4	-	0/4/27/29	0/2/2/2
7	SUC	D	501	-	-	0/12/51/51	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	605	3JY	O11-C10	-7.46	1.34	1.44
5	A	603	3JY	O11-C10	-7.43	1.34	1.44
5	A	603	3JY	C22-N21	-2.26	1.33	1.38
5	C	605	3JY	C20-C7	-2.24	1.50	1.53
5	A	603	3JY	C20-C7	-2.22	1.50	1.53
5	C	605	3JY	C22-N21	-2.17	1.33	1.38
5	C	605	3JY	P16-O18	2.20	1.53	1.49
5	A	603	3JY	O1-C2	3.86	1.34	1.24
5	C	605	3JY	O1-C2	3.88	1.34	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	605	3JY	C3-C2-N21	-6.90	119.55	125.35
5	A	603	3JY	C3-C2-N21	-6.89	119.57	125.35
7	D	501	SUC	C6'-C5'-C4'	-2.19	109.85	115.08
7	D	501	SUC	C1'-C2'-C3'	-2.14	107.18	114.44
5	C	605	3JY	C20-C7-C8	2.11	106.08	102.95
7	B	501	SUC	O1-C2'-C1'	2.22	116.74	109.62
5	C	605	3JY	C8-C9-C10	2.33	106.86	102.54
5	A	603	3JY	C20-C7-C8	2.42	106.53	102.95
5	A	603	3JY	C8-C9-C10	2.42	107.02	102.54
5	A	603	3JY	C10-C20-C7	2.95	108.49	102.49
5	C	605	3JY	C10-C20-C7	3.04	108.66	102.49
5	A	603	3JY	C2-N21-C22	7.59	121.49	115.16
5	C	605	3JY	C2-N21-C22	7.70	121.58	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	605	3JY	4	0
7	D	501	SUC	1	0

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, 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	551/555 (99%)	1.08	92 (16%) 2 1	41, 96, 151, 190	0
1	C	551/555 (99%)	1.34	135 (24%) 1 0	43, 113, 162, 182	0
2	B	412/444 (92%)	0.61	33 (8%) 15 10	41, 81, 127, 142	0
2	D	412/444 (92%)	0.85	55 (13%) 4 3	44, 92, 136, 160	0
3	E	33/38 (86%)	0.13	0 100 100	70, 97, 113, 152	0
3	F	33/38 (86%)	0.79	2 (6%) 25 18	82, 112, 131, 169	0
All	All	1992/2074 (96%)	0.98	317 (15%) 3 2	41, 93, 152, 190	0

All (317) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	134	SER	14.3
1	C	60	VAL	12.0
1	C	132	ILE	11.6
1	A	131	THR	11.1
1	C	135	ILE	10.8
1	C	142	ILE	9.6
1	C	133	PRO	9.5
1	C	50	ILE	9.2
2	D	10	VAL	8.8
1	A	142	ILE	8.6
1	C	67	ASP	7.9
1	A	134	SER	7.8
1	A	133	PRO	7.5
1	A	136	ASN	7.4
2	B	214	LEU	7.1
1	C	26	LEU	7.1
1	A	135	ILE	7.0
1	A	26	LEU	7.0
1	A	137	ASN	6.7

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Mol	Chain	Res	Type	RSRZ
1	C	28	GLU	6.4
1	C	25	PRO	6.3
1	C	24	TRP	6.1
1	C	138	GLU	6.1
1	A	138	GLU	5.9
1	C	17	ASP	5.9
1	A	28	GLU	5.7
1	C	131	THR	5.7
1	A	132	ILE	5.7
1	C	47	ILE	5.6
2	D	360	ALA	5.6
1	A	49	LYS	5.6
1	A	287	LYS	5.5
1	A	61	PHE	5.5
1	C	293	ILE	5.5
2	D	214	LEU	5.4
1	C	55	PRO	5.4
1	C	49	LYS	5.4
1	C	136	ASN	5.4
2	B	211	ARG	5.4
1	C	174	GLN	5.3
1	C	287	LYS	5.3
1	C	257	ILE	5.3
1	C	21	VAL	5.2
1	A	20	LYS	5.2
2	B	89	GLU	5.2
1	A	50	ILE	5.1
1	C	5	ILE	5.1
1	C	145	GLN	5.1
1	C	288	ALA	5.1
1	C	290	THR	5.1
1	A	27	THR	5.0
1	C	254	VAL	4.9
2	D	232	TYR	4.9
1	C	74	LEU	4.9
1	C	140	PRO	4.9
1	C	285	GLY	4.9
2	D	88	TRP	4.8
2	D	124	PHE	4.8
2	D	85	GLN	4.7
1	A	25	PRO	4.7
2	D	91	GLN	4.7

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Mol	Chain	Res	Type	RSRZ
2	D	116	PHE	4.7
1	A	251	SER	4.7
2	B	301	LEU	4.6
1	C	43	LYS	4.6
2	D	11	LYS	4.6
1	C	16	MET	4.6
1	C	23	GLN	4.5
2	B	4	PRO	4.5
1	A	47	ILE	4.5
2	B	212	TRP	4.5
1	C	66	LYS	4.4
1	A	286	THR	4.3
1	A	139	THR	4.3
1	A	193	LEU	4.3
1	C	228	LEU	4.3
2	D	357	MET	4.2
2	B	215	THR	4.2
1	A	21	VAL	4.2
1	A	288	ALA	4.2
1	C	193	LEU	4.2
1	C	58	THR	4.2
1	A	143	ARG	4.2
1	C	124	PHE	4.2
1	C	14	PRO	4.2
1	C	295	LEU	4.2
1	A	75	VAL	4.1
2	D	89	GLU	4.1
2	D	277	ARG	4.1
1	C	15	GLY	4.1
1	C	139	THR	4.0
1	C	210	LEU	4.0
1	C	22	LYS	4.0
1	C	141	GLY	4.0
1	A	73	LYS	4.0
1	C	61	PHE	4.0
1	A	62	ALA	4.0
1	C	73	LYS	3.9
2	B	250	ASP	3.9
1	A	144	TYR	3.9
1	C	59	PRO	3.9
1	C	144	TYR	3.9
1	C	346	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	63	ILE	3.8
1	C	102	LYS	3.8
2	D	359	GLY	3.8
1	C	18	GLY	3.8
1	A	448	ARG	3.8
1	C	151	GLN	3.8
2	D	318	TYR	3.7
1	C	286	THR	3.7
2	D	146	TYR	3.7
1	A	59	PRO	3.7
1	A	252	TRP	3.7
2	D	358	ARG	3.6
1	A	293	ILE	3.6
1	C	13	LYS	3.6
1	C	20	LYS	3.6
2	D	361	HIS	3.6
2	B	88	TRP	3.6
2	B	16	MET	3.6
1	A	71	TRP	3.6
2	D	215	THR	3.6
1	C	211	ARG	3.5
1	C	449	GLU	3.5
1	A	250	ASP	3.5
1	C	448	ARG	3.5
2	D	87	PHE	3.5
1	C	109	LEU	3.4
1	C	289	LEU	3.4
1	C	143	ARG	3.4
1	C	250	ASP	3.4
1	C	114	ALA	3.4
1	A	247	PRO	3.4
1	C	173	LYS	3.4
1	A	191	SER	3.4
2	B	12	LEU	3.4
1	A	290	THR	3.3
1	C	75	VAL	3.4
2	D	86	ASP	3.3
1	C	56	TYR	3.3
1	A	228	LEU	3.3
1	A	151	GLN	3.3
1	C	33	ALA	3.3
1	C	229	TRP	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	251	SER	3.2
2	D	159	ILE	3.2
2	D	195	ILE	3.2
2	B	6	GLU	3.2
2	D	16	MET	3.2
1	C	104	LYS	3.2
1	C	319	TYR	3.2
1	A	30	LYS	3.2
1	C	12	LEU	3.2
1	A	295	LEU	3.1
2	D	4	PRO	3.1
2	B	87	PHE	3.1
1	A	19	PRO	3.1
2	D	212	TRP	3.0
1	C	260	LEU	3.0
1	A	16	MET	3.0
2	B	86	ASP	3.0
1	C	283	LEU	3.0
1	C	32	LYS	3.0
2	B	14	PRO	3.0
1	A	145	GLN	3.0
2	B	5	ILE	3.0
2	D	238	LYS	3.0
2	D	233	GLU	3.0
1	C	137	ASN	2.9
1	C	259	LYS	2.9
1	C	195	ILE	2.9
2	D	422	LEU	2.9
2	D	176	PRO	2.9
1	A	289	LEU	2.9
2	B	425	LEU	2.9
1	C	11	LYS	2.9
1	A	130	PHE	2.9
1	C	223	LYS	2.9
1	C	207	GLN	2.8
1	A	37	ILE	2.8
1	C	188	TYR	2.8
2	D	92	LEU	2.8
1	C	4	PRO	2.8
2	D	354	TYR	2.8
1	C	252	TRP	2.8
1	A	56	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	554	ALA	2.8
1	A	51	GLY	2.8
1	A	452	LEU	2.7
1	A	226	PRO	2.7
2	D	90	VAL	2.7
1	A	271	TYR	2.7
2	D	240	THR	2.7
1	C	554	ALA	2.7
1	A	238	LYS	2.7
1	C	52	PRO	2.7
1	C	77	PHE	2.7
1	C	160	PHE	2.7
1	C	27	THR	2.7
2	D	426	TRP	2.7
2	B	195	ILE	2.7
1	C	19	PRO	2.6
1	C	146	TYR	2.6
1	C	294	PRO	2.6
2	D	95	PRO	2.6
1	A	17	ASP	2.6
2	D	15	GLY	2.6
2	D	169	GLU	2.6
1	A	141	GLY	2.6
1	A	128	THR	2.6
1	A	256	ASP	2.6
1	C	292	VAL	2.6
1	A	279	LEU	2.6
1	C	303	LEU	2.6
3	F	0	DT	2.5
1	C	78	ARG	2.5
1	C	130	PHE	2.5
1	A	52	PRO	2.5
1	A	60	VAL	2.5
1	A	120	LEU	2.5
1	A	127	TYR	2.5
1	C	232	TYR	2.5
1	C	115	TYR	2.5
2	B	10	VAL	2.5
1	A	200	THR	2.5
1	C	44	GLU	2.5
2	B	205	LEU	2.5
1	A	146	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	173	LYS	2.5
1	A	285	GLY	2.4
2	B	127	TYR	2.4
2	D	177	ASP	2.4
1	A	140	PRO	2.4
1	C	187	LEU	2.4
1	C	301	LEU	2.4
2	B	184	MET	2.4
2	B	193	LEU	2.4
1	C	184	MET	2.4
1	C	156	SER	2.4
1	A	254	VAL	2.4
1	C	318	TYR	2.3
2	B	400	THR	2.3
1	A	233	GLU	2.3
1	C	29	GLU	2.3
2	B	13	LYS	2.3
1	A	283	LEU	2.3
1	A	449	GLU	2.3
1	A	195	ILE	2.3
2	D	201	LYS	2.3
1	C	291	GLU	2.3
2	B	281	LYS	2.3
1	C	108	VAL	2.3
2	D	73	LYS	2.3
1	C	30	LYS	2.3
1	C	51	GLY	2.3
1	A	211	ARG	2.3
1	A	46	LYS	2.3
2	D	55	PRO	2.2
1	A	76	ASP	2.2
2	D	130	PHE	2.2
1	A	249	LYS	2.2
1	A	124	PHE	2.2
1	A	102	LYS	2.2
2	D	144	TYR	2.2
1	C	238	LYS	2.2
2	D	211	ARG	2.2
1	C	226	PRO	2.2
2	B	422	LEU	2.2
1	A	32	LYS	2.2
2	D	202	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	34	LEU	2.2
2	D	349	LEU	2.2
1	C	199	ARG	2.2
2	D	70	LYS	2.1
1	C	106	VAL	2.1
1	C	230	MET	2.1
1	C	10	VAL	2.1
2	D	127	TYR	2.1
2	B	171	PHE	2.1
1	C	183	TYR	2.1
1	C	120	LEU	2.1
1	C	277	ARG	2.1
1	A	192	ASP	2.1
1	A	453	GLY	2.1
1	C	284	ARG	2.1
1	C	325	LEU	2.1
2	D	32	LYS	2.1
1	A	29	GLU	2.1
1	C	178	ILE	2.1
1	C	279	LEU	2.1
2	B	204	GLU	2.1
1	A	241	VAL	2.1
1	A	291	GLU	2.1
1	C	302	GLU	2.1
3	F	37	DG	2.1
1	C	111	VAL	2.1
1	C	255	ASN	2.1
1	C	224	GLU	2.1
2	D	12	LEU	2.0
1	A	292	VAL	2.0
1	A	87	PHE	2.0
1	A	323	LYS	2.0
1	C	153	TRP	2.0
2	B	85	GLN	2.0
1	C	209	LEU	2.0
2	D	198	HIS	2.0
2	D	47	ILE	2.0
1	A	42	GLU	2.0
1	C	308	GLU	2.0
2	D	66	LYS	2.0
2	D	197	GLN	2.0
1	A	248	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	397	THR	2.0
1	C	452	LEU	2.0
1	C	313	PRO	2.0
2	B	275	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	OMC	F	8	21/22	0.92	0.25	-	95,103,106,118	0
3	OMC	E	8	21/22	0.94	0.23	-	67,73,76,90	0
3	OMC	E	6	21/22	0.97	0.20	-	82,91,95,98	0
3	OMC	F	6	21/22	0.90	0.24	-	85,98,111,120	0

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, 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	LLDF	B-factors(Å ²)	Q<0.9
6	SO4	B	505	5/5	0.81	0.40	4.12	78,78,84,111	0
6	SO4	B	504	5/5	0.85	0.39	3.22	87,98,102,121	0
6	SO4	C	604	5/5	0.88	0.24	0.69	84,92,112,112	0
4	MG	C	601	1/1	0.96	0.28	-0.07	122,122,122,122	0
4	MG	A	601	1/1	0.97	0.20	-0.18	114,114,114,114	0
5	3JY	A	603	23/24	0.94	0.20	-0.39	103,107,123,129	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	SUC	B	501	23/23	0.89	0.19	-0.70	67,84,107,109	0
6	SO4	B	502	5/5	0.85	0.21	-0.86	78,79,85,101	0
5	3JY	C	605	23/24	0.84	0.24	-0.87	98,119,137,145	0
6	SO4	A	605	5/5	0.95	0.12	-1.43	98,102,110,116	0
7	SUC	D	501	23/23	0.93	0.15	-2.02	82,96,102,104	0
4	MG	A	604	1/1	0.92	0.14	-	70,70,70,70	0
4	MG	A	602	1/1	0.84	0.15	-	114,114,114,114	0
6	SO4	B	503	5/5	0.85	0.17	-	94,100,109,113	0
4	MG	C	603	1/1	0.56	0.14	-	172,172,172,172	0
4	MG	C	602	1/1	0.95	0.19	-	70,70,70,70	0

6.5 Other polymers

There are no such residues in this entry.