



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:55 am GMT

PDB ID : 5A03
Title : Crystal structure of aldose-aldose oxidoreductase from *Caulobacter crescentus* complexed with xylose
Authors : Taberman, H.; Rouvinen, J.; Parkkinen, T.
Deposited on : 2015-04-17
Resolution : 1.85 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

<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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

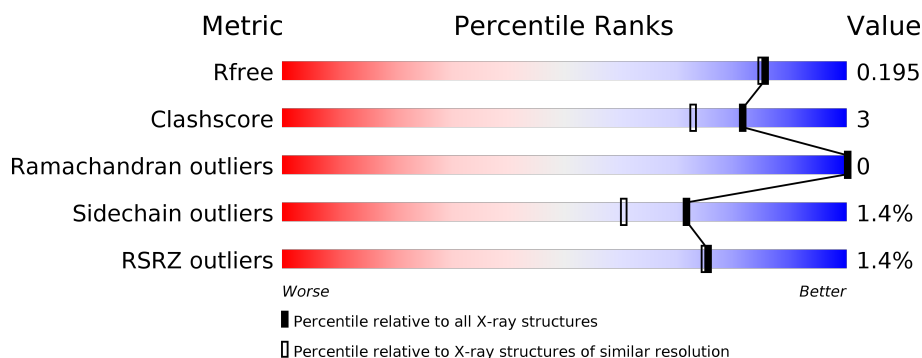
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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}	100719	2964 (1.86-1.82)
Clashscore	112137	3197 (1.86-1.82)
Ramachandran outliers	110173	3164 (1.86-1.82)
Sidechain outliers	110143	3165 (1.86-1.82)
RSRZ outliers	101464	2973 (1.86-1.82)

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	339	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>6%</div> <div>.</div> </div> </div>
1	B	339	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>8%</div> <div>..</div> </div> </div>
1	C	339	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>6%</div> <div>.</div> </div> </div>
1	D	339	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>6%</div> <div>.</div> </div> </div>
1	E	339	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>5%</div> <div>.</div> </div> </div>
1	F	339	<div> <div>%</div> <div> <div></div> <div>93%</div> <div>6%</div> <div>.</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
3	XYP	C	1341	-	-	-	X
3	XYP	D	1341	-	-	-	X
3	XYP	E	1343	-	-	-	X
4	SO4	A	1345	-	-	-	X
4	SO4	A	1346	-	-	-	X
4	SO4	C	1343	-	-	-	X
4	SO4	D	1346	-	-	-	X
5	XYS	E	1344	-	-	-	X
6	DIO	D	1343	-	-	-	X

2 Entry composition [i](#)

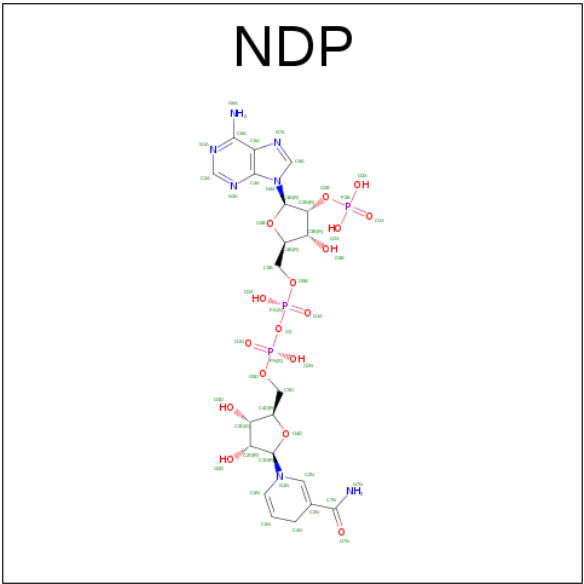
There are 7 unique types of molecules in this entry. The entry contains 17880 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALDOSE-ALDOSE OXIDOREDUCTASE.

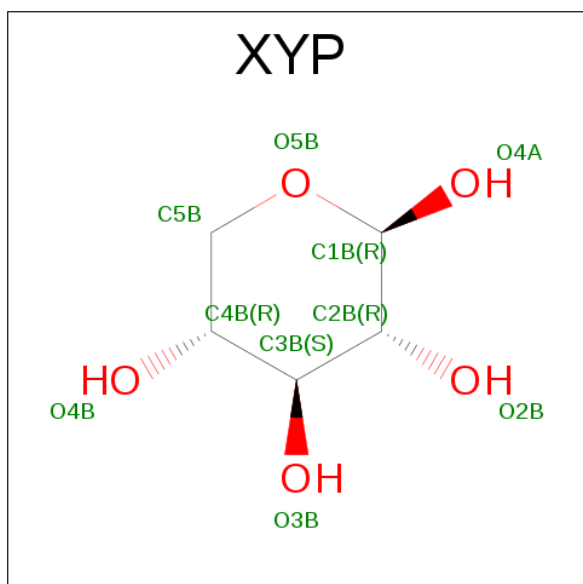
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2593	1626	471	482	14			
1	B	335	Total	C	N	O	S	0	0	0
			2593	1626	471	482	14			
1	C	336	Total	C	N	O	S	0	0	0
			2597	1628	472	483	14			
1	D	335	Total	C	N	O	S	0	0	0
			2593	1626	471	482	14			
1	E	335	Total	C	N	O	S	0	0	0
			2593	1626	471	482	14			
1	F	335	Total	C	N	O	S	0	1	0
			2604	1632	475	483	14			

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is SUGAR (BETA-D-XYLOPYRANOSE) (three-letter code: XYP) (formula: $C_5H_{10}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		
3	A	1	Total	C	O	0	0
			10	5	5		
3	A	1	Total	C	O	0	0
			10	5	5		
3	A	1	Total	C	O	0	0
			10	5	5		
3	B	1	Total	C	O	0	0
			10	5	5		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			10	5	5		
3	C	1	Total	C	O	0	0
			10	5	5		
3	D	1	Total	C	O	0	0
			10	5	5		
3	D	1	Total	C	O	0	0
			10	5	5		
3	E	1	Total	C	O	0	0
			10	5	5		
3	E	1	Total	C	O	0	0
			10	5	5		
3	E	1	Total	C	O	0	0
			10	5	5		
3	F	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



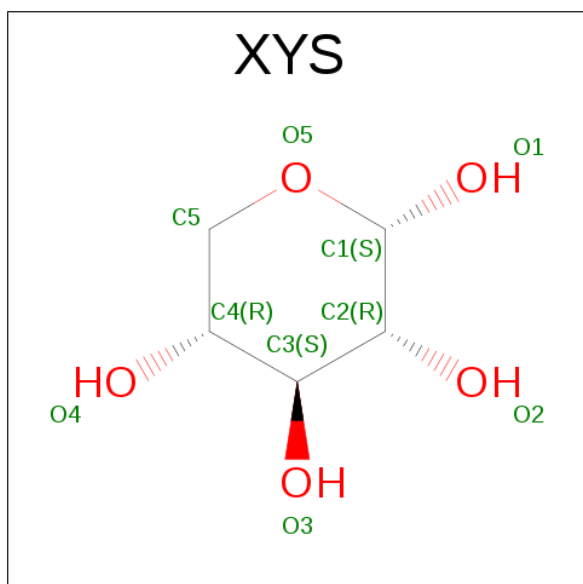
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

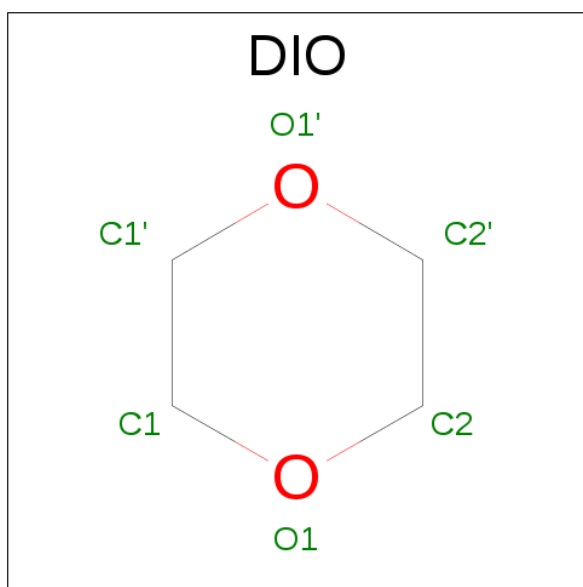
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is SUGAR (XYLOPYRANOSE) (three-letter code: XYS) (formula: C₅H₁₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			10	5	5		
5	E	1	Total	C	O	0	0
			10	5	5		

- Molecule 6 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C₄H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			6	4	2		
6	D	1	Total	C	O	0	0
			6	4	2		

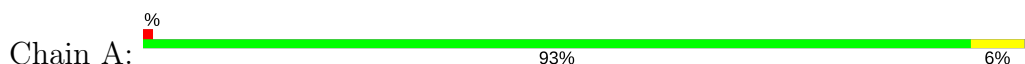
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	374	Total	O	0	0
			374	374		
7	B	286	Total	O	0	0
			286	286		
7	C	303	Total	O	0	0
			303	303		
7	D	285	Total	O	0	0
			285	285		
7	E	275	Total	O	0	0
			275	275		
7	F	289	Total	O	0	0
			289	289		

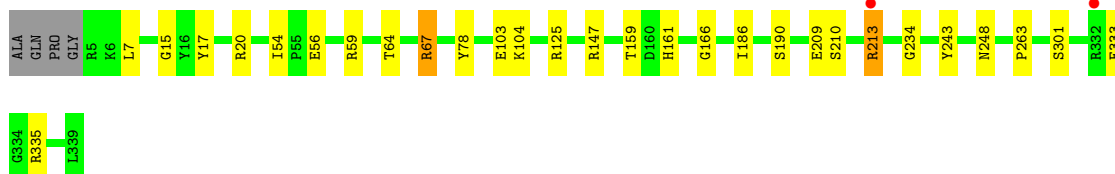
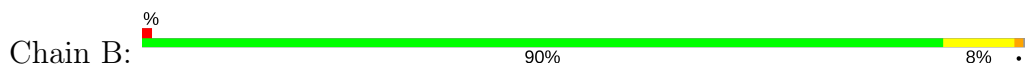
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

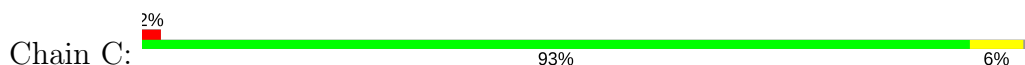
- Molecule 1: ALDOSE-ALDOSE OXIDOREDUCTASE



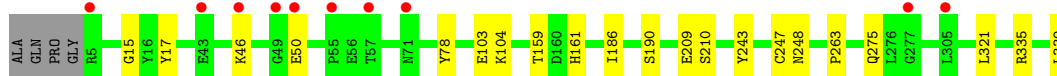
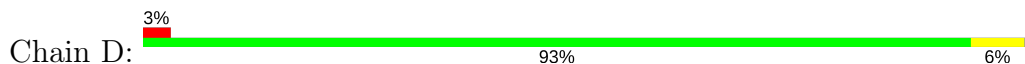
- Molecule 1: ALDOSE-ALDOSE OXIDOREDUCTASE



- Molecule 1: ALDOSE-ALDOSE OXIDOREDUCTASE



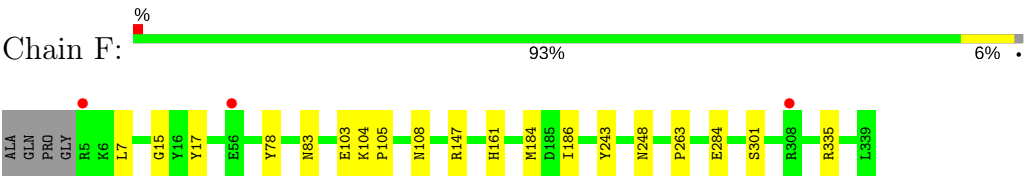
- Molecule 1: ALDOSE-ALDOSE OXIDOREDUCTASE



- Molecule 1: ALDOSE-ALDOSE OXIDOREDUCTASE



● Molecule 1: ALDOSE-ALDOSE OXIDOREDUCTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.06Å 153.48Å 107.33Å 90.00° 109.42° 90.00°	Depositor
Resolution (Å)	49.99 – 1.85 49.99 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.4 (49.99-1.85) 97.5 (49.99-1.85)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 1.84Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.167 , 0.195 0.166 , 0.195	Depositor DCC
R_{free} test set	12801 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17880	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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: XYP, NDP, DIO, XYS, 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	0.39	0/2648	0.53	0/3586
1	B	0.35	0/2648	0.52	0/3586
1	C	0.35	0/2652	0.51	0/3591
1	D	0.35	0/2648	0.51	0/3586
1	E	0.37	0/2648	0.52	0/3586
1	F	0.38	0/2659	0.52	0/3600
All	All	0.36	0/15903	0.52	0/21535

There are no bond length outliers.

There are no bond angle outliers.

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	2593	0	2580	16	0
1	B	2593	0	2580	22	0
1	C	2597	0	2583	15	0
1	D	2593	0	2580	12	0
1	E	2593	0	2580	11	0
1	F	2604	0	2592	12	0
2	A	48	0	26	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	48	0	26	5	0
2	C	48	0	26	6	0
2	D	48	0	26	5	0
2	E	48	0	26	7	0
2	F	48	0	26	5	0
3	A	40	0	40	6	0
3	B	10	0	10	2	0
3	C	20	0	20	2	0
3	D	20	0	20	2	0
3	E	30	0	30	5	0
3	F	10	0	10	2	0
4	A	10	0	0	0	0
4	C	5	0	0	0	0
4	D	10	0	0	0	0
4	E	15	0	0	0	0
4	F	5	0	0	0	0
5	B	10	0	10	0	0
5	E	10	0	10	0	0
6	D	12	0	16	1	0
7	A	374	0	0	3	2
7	B	286	0	0	4	0
7	C	303	0	0	5	0
7	D	285	0	0	0	0
7	E	275	0	0	0	0
7	F	289	0	0	3	2
All	All	17880	0	15817	97	2

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 3.

All (97) 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:1340:NDP:H42N	3:B:1341:XYP:H1B	1.46	0.95
2:D:1340:NDP:H42N	3:D:1341:XYP:H1B	1.49	0.94
2:F:1340:NDP:H42N	3:F:1341:XYP:H1B	1.50	0.94
2:E:1340:NDP:H42N	3:E:1342:XYP:H1B	1.48	0.93
2:C:1340:NDP:H42N	3:C:1342:XYP:H1B	1.58	0.84
2:A:1340:NDP:H42N	3:A:1341:XYP:H1B	1.59	0.83
1:E:213:ARG:HE	3:E:1343:XYP:H5B1	1.49	0.78
1:E:40:GLY:HA3	3:E:1341:XYP:H5B1	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:TYR:CD1	2:C:1340:NDP:H41N	2.24	0.72
1:A:17:TYR:CD1	2:A:1340:NDP:H41N	2.25	0.72
1:A:147:ARG:NH2	7:A:2187:HOH:O	2.23	0.71
1:C:175:ARG:NH2	7:C:2191:HOH:O	2.24	0.70
1:E:17:TYR:CD1	2:E:1340:NDP:H41N	2.29	0.68
1:B:147:ARG:NH2	7:B:2149:HOH:O	2.27	0.67
1:D:17:TYR:CD1	2:D:1340:NDP:H41N	2.30	0.67
1:F:17:TYR:CD1	2:F:1340:NDP:H41N	2.29	0.67
7:A:2184:HOH:O	1:B:20:ARG:NH2	2.29	0.65
1:A:44:LYS:HZ3	3:A:1343:XYP:H1B	1.63	0.64
1:C:147:ARG:NH2	7:C:2150:HOH:O	2.32	0.63
1:C:5:ARG:NH2	7:C:2002:HOH:O	2.33	0.61
1:C:335:ARG:NH2	7:C:2293:HOH:O	2.32	0.61
1:B:67:ARG:NH1	7:B:2069:HOH:O	2.05	0.61
2:A:1340:NDP:H3B	3:A:1343:XYP:H3B	1.82	0.60
1:F:15:GLY:HA3	2:F:1340:NDP:O5B	2.00	0.60
1:D:15:GLY:HA3	2:D:1340:NDP:O5B	2.02	0.59
1:A:15:GLY:HA3	2:A:1340:NDP:O5B	2.04	0.58
2:D:1340:NDP:C4N	3:D:1341:XYP:H1B	2.31	0.56
1:C:14:LEU:HD22	1:C:39:SER:HB2	1.87	0.55
1:A:161:HIS:HB3	1:A:186:ILE:HG13	1.89	0.55
1:B:333:GLU:OE1	1:B:335:ARG:NE	2.37	0.54
1:E:161:HIS:HB3	1:E:186:ILE:HG13	1.88	0.54
2:F:1340:NDP:C4N	3:F:1341:XYP:H1B	2.32	0.54
1:B:17:TYR:CD1	2:B:1340:NDP:H41N	2.43	0.54
1:E:15:GLY:HA3	2:E:1340:NDP:O5B	2.07	0.53
1:B:213:ARG:HD3	7:B:2204:HOH:O	2.09	0.53
1:A:335:ARG:HA	1:E:335:ARG:HA	1.90	0.53
1:F:161:HIS:HB3	1:F:186:ILE:HG13	1.91	0.53
1:A:44:LYS:NZ	3:A:1343:XYP:H1B	2.24	0.53
2:E:1340:NDP:C4N	3:E:1342:XYP:H1B	2.32	0.52
1:F:147[A]:ARG:NH2	7:F:2148:HOH:O	2.38	0.52
1:F:103:GLU:OE1	2:F:1340:NDP:H2N	2.10	0.51
1:F:147[B]:ARG:HG3	7:F:2151:HOH:O	2.10	0.51
2:A:1340:NDP:C4N	3:A:1341:XYP:H1B	2.36	0.51
1:B:54:ILE:O	1:B:59:ARG:NH1	2.34	0.51
1:D:103:GLU:OE1	2:D:1340:NDP:H2N	2.11	0.50
1:B:234:GLY:HA3	6:D:1343:DIO:H2'1	1.94	0.50
2:B:1340:NDP:C4N	3:B:1341:XYP:H1B	2.31	0.49
1:B:161:HIS:HB3	1:B:186:ILE:HG13	1.93	0.49
1:A:144:LYS:HG3	7:A:2183:HOH:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1340:NDP:C4N	3:C:1342:XYP:H1B	2.35	0.49
1:B:15:GLY:HA3	2:B:1340:NDP:O5B	2.13	0.48
1:B:335:ARG:HA	1:D:335:ARG:HA	1.94	0.48
1:A:141:GLU:CD	1:B:20:ARG:HH22	2.17	0.47
1:A:141:GLU:OE1	1:B:20:ARG:NH2	2.43	0.47
1:C:335:ARG:HA	1:F:335:ARG:HA	1.97	0.47
1:F:248:ASN:O	1:F:263:PRO:HA	2.14	0.47
1:B:103:GLU:OE1	2:B:1340:NDP:H2N	2.15	0.46
1:E:209:GLU:HG2	1:E:210:SER:N	2.29	0.46
1:C:161:HIS:HB3	1:C:186:ILE:HG13	1.98	0.46
1:C:103:GLU:OE1	2:C:1340:NDP:H2N	2.16	0.46
1:A:103:GLU:OE1	2:A:1340:NDP:H2N	2.16	0.46
1:A:248:ASN:O	1:A:263:PRO:HA	2.15	0.46
1:C:169:LYS:HD3	1:C:169:LYS:HA	1.76	0.46
1:D:248:ASN:O	1:D:263:PRO:HA	2.15	0.46
2:A:1340:NDP:C3B	3:A:1343:XYP:H3B	2.45	0.46
1:B:209:GLU:HG2	1:B:210:SER:N	2.31	0.46
1:D:209:GLU:HG2	1:D:210:SER:N	2.31	0.45
1:F:284:GLU:OE1	7:F:2250:HOH:O	2.21	0.45
1:C:15:GLY:HA3	2:C:1340:NDP:O5B	2.16	0.45
1:B:159:THR:HG23	1:B:190:SER:HB3	1.99	0.45
1:E:103:GLU:OE1	2:E:1340:NDP:H2N	2.17	0.45
1:C:17:TYR:CE1	2:C:1340:NDP:H41N	2.53	0.44
1:C:248:ASN:O	1:C:263:PRO:HA	2.17	0.44
1:E:248:ASN:O	1:E:263:PRO:HA	2.18	0.43
2:E:1340:NDP:O5D	2:E:1340:NDP:H6N	2.18	0.43
1:B:248:ASN:O	1:B:263:PRO:HA	2.18	0.43
1:A:39:SER:O	1:A:61:SER:HA	2.19	0.43
1:C:247:CYS:HB3	7:C:2232:HOH:O	2.19	0.43
1:D:159:THR:HG23	1:D:190:SER:HB3	2.01	0.42
1:B:56:GLU:HA	1:B:59:ARG:HD3	2.01	0.42
1:D:46:LYS:NZ	1:D:50:GLU:OE2	2.47	0.42
1:A:17:TYR:CE1	2:A:1340:NDP:H41N	2.55	0.42
1:F:108:ASN:HA	1:F:184:MET:HE1	2.02	0.42
7:B:2226:HOH:O	1:D:247:CYS:HB3	2.19	0.41
1:C:167:ASP:HA	1:C:168:PRO:HD2	1.98	0.41
1:D:321:LEU:HA	1:D:321:LEU:HD13	1.92	0.41
1:E:213:ARG:HE	3:E:1343:XYP:C5B	2.26	0.41
2:E:1340:NDP:H3B	2:E:1340:NDP:N3A	2.36	0.41
1:D:161:HIS:HB3	1:D:186:ILE:HG13	2.03	0.41
1:A:224:ILE:HD11	1:E:155:ARG:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:LEU:HD12	1:B:301:SER:HA	2.02	0.41
1:A:276:LEU:O	1:B:166:GLY:HA3	2.21	0.41
1:F:7:LEU:HD12	1:F:301:SER:HA	2.04	0.40
1:B:64:THR:O	1:B:67:ARG:HD3	2.20	0.40
1:D:339:LEU:HA	1:D:339:LEU:HD23	1.89	0.40
1:B:125:ARG:HD3	1:B:125:ARG:HA	1.91	0.40
1:F:83:ASN:OD1	1:F:105:PRO:HD2	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:2138:HOH:O	7:F:2289:HOH:O[2_656]	2.12	0.08
7:A:2220:HOH:O	7:F:2016:HOH:O[2_656]	2.18	0.02

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	333/339 (98%)	324 (97%)	9 (3%)	0	100	100
1	B	333/339 (98%)	325 (98%)	8 (2%)	0	100	100
1	C	334/339 (98%)	326 (98%)	8 (2%)	0	100	100
1	D	333/339 (98%)	326 (98%)	7 (2%)	0	100	100
1	E	333/339 (98%)	327 (98%)	6 (2%)	0	100	100
1	F	334/339 (98%)	325 (97%)	9 (3%)	0	100	100
All	All	2000/2034 (98%)	1953 (98%)	47 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	270/272 (99%)	267 (99%)	3 (1%)	78	70
1	B	270/272 (99%)	265 (98%)	5 (2%)	62	47
1	C	270/272 (99%)	266 (98%)	4 (2%)	70	57
1	D	270/272 (99%)	266 (98%)	4 (2%)	70	57
1	E	270/272 (99%)	267 (99%)	3 (1%)	78	70
1	F	271/272 (100%)	268 (99%)	3 (1%)	78	70
All	All	1621/1632 (99%)	1599 (99%)	22 (1%)	71	60

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	TYR
1	A	104	LYS
1	A	243	TYR
1	B	67	ARG
1	B	78	TYR
1	B	104	LYS
1	B	213	ARG
1	B	243	TYR
1	C	5	ARG
1	C	78	TYR
1	C	104	LYS
1	C	243	TYR
1	D	78	TYR
1	D	104	LYS
1	D	243	TYR
1	D	275	GLN
1	E	78	TYR
1	E	104	LYS
1	E	243	TYR
1	F	78	TYR
1	F	104	LYS
1	F	243	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

32 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NDP	A	1340	-	43,52,52	1.76	5 (11%)	49,80,80	1.29	6 (12%)
3	XYP	A	1341	-	10,10,10	0.50	0	14,14,14	1.17	1 (7%)
3	XYP	A	1342	-	10,10,10	0.65	0	14,14,14	0.81	0
3	XYP	A	1343	-	10,10,10	0.74	0	14,14,14	1.02	1 (7%)
3	XYP	A	1344	-	10,10,10	0.72	0	14,14,14	0.78	0
4	SO4	A	1345	-	4,4,4	0.23	0	6,6,6	0.11	0
4	SO4	A	1346	-	4,4,4	0.20	0	6,6,6	0.14	0
2	NDP	B	1340	-	43,52,52	2.25	5 (11%)	49,80,80	1.26	7 (14%)
3	XYP	B	1341	-	10,10,10	0.66	0	14,14,14	1.36	2 (14%)
5	XYS	B	1342	-	10,10,10	1.65	1 (10%)	14,14,14	1.02	1 (7%)
2	NDP	C	1340	-	43,52,52	2.17	5 (11%)	49,80,80	1.27	5 (10%)
3	XYP	C	1341	-	10,10,10	0.63	0	14,14,14	1.44	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	XYP	C	1342	-	10,10,10	0.68	0	14,14,14	0.95	1 (7%)
4	SO4	C	1343	-	4,4,4	0.17	0	6,6,6	0.09	0
2	NDP	D	1340	-	43,52,52	2.19	7 (16%)	49,80,80	1.27	5 (10%)
3	XYP	D	1341	-	10,10,10	0.70	0	14,14,14	1.17	1 (7%)
3	XYP	D	1342	-	10,10,10	0.65	0	14,14,14	1.14	1 (7%)
6	DIO	D	1343	-	6,6,6	0.46	0	6,6,6	0.83	0
6	DIO	D	1344	-	6,6,6	0.46	0	6,6,6	0.59	0
4	SO4	D	1345	-	4,4,4	0.13	0	6,6,6	0.13	0
4	SO4	D	1346	-	4,4,4	0.20	0	6,6,6	0.09	0
2	NDP	E	1340	-	43,52,52	2.14	5 (11%)	49,80,80	1.29	7 (14%)
3	XYP	E	1341	-	10,10,10	0.91	0	14,14,14	1.20	1 (7%)
3	XYP	E	1342	-	10,10,10	0.68	0	14,14,14	1.07	2 (14%)
3	XYP	E	1343	-	10,10,10	0.86	0	14,14,14	1.80	2 (14%)
5	XYS	E	1344	-	10,10,10	1.36	1 (10%)	14,14,14	1.59	3 (21%)
4	SO4	E	1345	-	4,4,4	0.19	0	6,6,6	0.09	0
4	SO4	E	1346	-	4,4,4	0.19	0	6,6,6	0.17	0
4	SO4	E	1347	-	4,4,4	0.15	0	6,6,6	0.10	0
2	NDP	F	1340	-	43,52,52	2.12	7 (16%)	49,80,80	1.33	5 (10%)
3	XYP	F	1341	-	10,10,10	0.68	0	14,14,14	1.29	1 (7%)
4	SO4	F	1342	-	4,4,4	0.26	0	6,6,6	0.16	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
2	NDP	A	1340	-	-	0/30/77/77	0/5/5/5
3	XYP	A	1341	-	-	0/0/17/17	0/1/1/1
3	XYP	A	1342	-	-	0/0/17/17	0/1/1/1
3	XYP	A	1343	-	-	0/0/17/17	0/1/1/1
3	XYP	A	1344	-	-	0/0/17/17	0/1/1/1
4	SO4	A	1345	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1346	-	-	0/0/0/0	0/0/0/0
2	NDP	B	1340	-	-	0/30/77/77	0/5/5/5
3	XYP	B	1341	-	-	0/0/17/17	0/1/1/1
5	XYS	B	1342	-	-	0/0/17/17	0/1/1/1
2	NDP	C	1340	-	-	0/30/77/77	0/5/5/5
3	XYP	C	1341	-	-	0/0/17/17	0/1/1/1
3	XYP	C	1342	-	-	0/0/17/17	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	C	1343	-	-	0/0/0/0	0/0/0/0
2	NDP	D	1340	-	-	0/30/77/77	0/5/5/5
3	XYP	D	1341	-	-	0/0/17/17	0/1/1/1
3	XYP	D	1342	-	-	0/0/17/17	0/1/1/1
6	DIO	D	1343	-	-	0/0/6/6	0/1/1/1
6	DIO	D	1344	-	-	0/0/6/6	0/1/1/1
4	SO4	D	1345	-	-	0/0/0/0	0/0/0/0
4	SO4	D	1346	-	-	0/0/0/0	0/0/0/0
2	NDP	E	1340	-	-	0/30/77/77	0/5/5/5
3	XYP	E	1341	-	-	0/0/17/17	0/1/1/1
3	XYP	E	1342	-	-	0/0/17/17	0/1/1/1
3	XYP	E	1343	-	-	0/0/17/17	0/1/1/1
5	XYS	E	1344	-	-	0/0/17/17	0/1/1/1
4	SO4	E	1345	-	-	0/0/0/0	0/0/0/0
4	SO4	E	1346	-	-	0/0/0/0	0/0/0/0
4	SO4	E	1347	-	-	0/0/0/0	0/0/0/0
2	NDP	F	1340	-	-	0/30/77/77	0/5/5/5
3	XYP	F	1341	-	-	0/0/17/17	0/1/1/1
4	SO4	F	1342	-	-	0/0/0/0	0/0/0/0

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1342	XYS	O5-C1	-4.78	1.36	1.43
5	E	1344	XYS	O5-C1	-3.98	1.37	1.43
2	F	1340	NDP	O2B-C2B	-3.76	1.29	1.44
2	A	1340	NDP	O2B-C2B	-3.39	1.31	1.44
2	E	1340	NDP	O2B-C2B	-3.34	1.31	1.44
2	C	1340	NDP	O2B-C2B	-3.23	1.31	1.44
2	D	1340	NDP	O2B-C2B	-3.22	1.31	1.44
2	B	1340	NDP	O2B-C2B	-3.03	1.32	1.44
2	E	1340	NDP	C2A-N1A	2.01	1.37	1.33
2	C	1340	NDP	C2A-N1A	2.01	1.37	1.33
2	D	1340	NDP	C4A-N3A	2.09	1.38	1.35
2	F	1340	NDP	C7N-N7N	2.15	1.39	1.33
2	F	1340	NDP	C3D-C4D	2.16	1.58	1.53
2	D	1340	NDP	C3D-C4D	2.19	1.58	1.53
2	A	1340	NDP	C4A-N3A	2.22	1.38	1.35
2	D	1340	NDP	C7N-N7N	2.23	1.39	1.33
2	F	1340	NDP	C2A-N1A	2.28	1.38	1.33
2	C	1340	NDP	C7N-N7N	2.30	1.39	1.33
2	E	1340	NDP	O4B-C1B	2.38	1.44	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1340	NDP	C2A-N1A	2.39	1.38	1.33
2	B	1340	NDP	C7N-N7N	2.40	1.40	1.33
2	F	1340	NDP	O4B-C1B	2.40	1.44	1.41
2	D	1340	NDP	C2A-N1A	2.45	1.38	1.33
2	B	1340	NDP	C2A-N1A	2.63	1.38	1.33
2	E	1340	NDP	PN-O5D	4.10	1.76	1.59
2	A	1340	NDP	PN-O5D	4.10	1.76	1.59
2	B	1340	NDP	PN-O5D	4.12	1.76	1.59
2	C	1340	NDP	PN-O5D	4.15	1.76	1.59
2	D	1340	NDP	PN-O5D	4.52	1.78	1.59
2	F	1340	NDP	PN-O5D	4.66	1.79	1.59
2	A	1340	NDP	P2B-O2B	8.18	1.73	1.59
2	F	1340	NDP	P2B-O2B	10.36	1.77	1.59
2	E	1340	NDP	P2B-O2B	11.11	1.79	1.59
2	D	1340	NDP	P2B-O2B	11.34	1.79	1.59
2	C	1340	NDP	P2B-O2B	11.39	1.79	1.59
2	B	1340	NDP	P2B-O2B	11.97	1.80	1.59

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1343	XYP	C5B-O5B-C1B	-5.49	103.29	112.80
3	C	1341	XYP	C4B-C3B-C2B	-4.14	103.66	110.88
3	E	1341	XYP	C5B-O5B-C1B	-3.73	106.35	112.80
3	B	1341	XYP	C5B-O5B-C1B	-3.59	106.58	112.80
3	A	1341	XYP	C5B-O5B-C1B	-3.47	106.79	112.80
2	F	1340	NDP	C4B-O4B-C1B	-3.45	106.10	109.77
3	F	1341	XYP	C5B-O5B-C1B	-3.27	107.15	112.80
2	D	1340	NDP	C4B-O4B-C1B	-3.15	106.42	109.77
3	D	1341	XYP	C5B-O5B-C1B	-3.04	107.53	112.80
2	A	1340	NDP	C4B-O4B-C1B	-3.00	106.57	109.77
2	E	1340	NDP	C4B-O4B-C1B	-2.72	106.88	109.77
3	E	1342	XYP	C5B-O5B-C1B	-2.65	108.22	112.80
3	D	1342	XYP	C4B-C3B-C2B	-2.57	106.39	110.88
3	A	1343	XYP	C5B-O5B-C1B	-2.53	108.42	112.80
2	C	1340	NDP	C4B-O4B-C1B	-2.47	107.14	109.77
2	D	1340	NDP	O2B-P2B-O1X	-2.43	99.74	109.26
2	A	1340	NDP	C3N-C2N-N1N	-2.38	119.62	123.08
3	E	1342	XYP	C1B-C2B-C3B	-2.38	106.35	110.65
2	E	1340	NDP	O2B-P2B-O1X	-2.37	99.97	109.26
2	B	1340	NDP	C4B-O4B-C1B	-2.31	107.31	109.77
2	B	1340	NDP	O2B-P2B-O1X	-2.30	100.24	109.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1340	NDP	C2A-N1A-C6A	-2.25	114.84	118.77
2	C	1340	NDP	C5B-C4B-C3B	-2.24	106.75	115.29
2	B	1340	NDP	C2A-N1A-C6A	-2.21	114.91	118.77
2	D	1340	NDP	C3N-C2N-N1N	-2.16	119.95	123.08
2	F	1340	NDP	C5B-C4B-C3B	-2.14	107.13	115.29
3	C	1342	XYP	C5B-O5B-C1B	-2.14	109.10	112.80
2	C	1340	NDP	O2B-P2B-O1X	-2.13	100.92	109.26
2	E	1340	NDP	O7N-C7N-N7N	-2.12	117.77	122.92
2	A	1340	NDP	O2B-P2B-O1X	-2.12	100.96	109.26
2	C	1340	NDP	O2N-PN-O5D	-2.10	98.22	108.14
2	F	1340	NDP	O2B-P2B-O1X	-2.09	101.06	109.26
2	E	1340	NDP	C5B-C4B-C3B	-2.09	107.34	115.29
2	B	1340	NDP	O7N-C7N-N7N	-2.08	117.87	122.92
2	E	1340	NDP	O5D-PN-O1N	-2.07	100.91	109.25
2	D	1340	NDP	C2A-N1A-C6A	-2.07	115.15	118.77
2	E	1340	NDP	C2A-N1A-C6A	-2.05	115.17	118.77
2	A	1340	NDP	C2A-N1A-C6A	-2.03	115.23	118.77
2	B	1340	NDP	O2N-PN-O1N	2.02	122.73	112.28
3	B	1341	XYP	O5B-C1B-C2B	2.07	112.08	109.31
2	A	1340	NDP	O2N-PN-O1N	2.09	123.10	112.28
3	E	1343	XYP	C5B-C4B-C3B	2.09	112.30	109.65
2	B	1340	NDP	N3A-C2A-N1A	2.18	130.75	128.86
2	C	1340	NDP	O3X-P2B-O2X	2.38	117.20	107.61
2	A	1340	NDP	O3X-P2B-O2X	2.44	117.45	107.61
2	B	1340	NDP	O3X-P2B-O2X	2.46	117.56	107.61
2	F	1340	NDP	O3X-P2B-O2X	2.48	117.60	107.61
2	D	1340	NDP	O3X-P2B-O2X	2.50	117.70	107.61
2	E	1340	NDP	O3X-P2B-O2X	2.53	117.82	107.61
5	B	1342	XYS	C5-O5-C1	2.71	117.50	112.80
5	E	1344	XYS	O5-C5-C4	2.92	115.37	110.79
5	E	1344	XYS	C5-O5-C1	3.08	118.14	112.80
5	E	1344	XYS	O5-C1-C2	3.45	113.93	109.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1340	NDP	8	0
3	A	1341	XYP	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1343	XYP	4	0
2	B	1340	NDP	5	0
3	B	1341	XYP	2	0
2	C	1340	NDP	6	0
3	C	1342	XYP	2	0
2	D	1340	NDP	5	0
3	D	1341	XYP	2	0
6	D	1343	DIO	1	0
2	E	1340	NDP	7	0
3	E	1341	XYP	1	0
3	E	1342	XYP	2	0
3	E	1343	XYP	2	0
2	F	1340	NDP	5	0
3	F	1341	XYP	2	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	335/339 (98%)	-0.34	2 (0%) 89 89	14, 19, 30, 50	0
1	B	335/339 (98%)	-0.16	2 (0%) 89 89	15, 23, 36, 53	0
1	C	336/339 (99%)	-0.16	6 (1%) 69 67	14, 23, 36, 53	0
1	D	335/339 (98%)	-0.17	10 (2%) 51 47	15, 22, 37, 52	0
1	E	335/339 (98%)	-0.06	5 (1%) 74 73	14, 21, 33, 46	0
1	F	335/339 (98%)	-0.14	3 (0%) 84 84	13, 20, 35, 52	0
All	All	2011/2034 (98%)	-0.17	28 (1%) 75 75	13, 21, 35, 53	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	5	ARG	5.1
1	C	4	GLY	5.1
1	A	5	ARG	4.5
1	D	5	ARG	4.3
1	D	43	GLU	3.5
1	D	50	GLU	3.5
1	D	277	GLY	3.1
1	D	49	GLY	2.9
1	F	56	GLU	2.9
1	E	57	THR	2.7
1	A	307	GLY	2.7
1	C	5	ARG	2.7
1	E	46	LYS	2.6
1	B	332	ARG	2.6
1	D	55	PRO	2.4
1	E	5	ARG	2.3
1	C	47	THR	2.3
1	E	50	GLU	2.3
1	D	57	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	214	SER	2.2
1	F	308	ARG	2.2
1	C	335	ARG	2.2
1	C	72	PRO	2.1
1	D	305	LEU	2.1
1	D	46	LYS	2.1
1	E	277	GLY	2.1
1	D	71	ASN	2.1
1	B	213	ARG	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, 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	DIO	D	1343	6/6	0.82	0.27	33.89	36,38,42,44	0
4	SO4	A	1346	5/5	0.97	0.20	8.14	37,42,49,50	0
3	XYP	E	1343	10/10	0.78	0.20	4.72	28,39,42,46	0
4	SO4	D	1346	5/5	0.93	0.21	4.42	50,61,64,69	0
4	SO4	C	1343	5/5	0.98	0.18	3.85	32,41,42,43	0
3	XYP	C	1341	10/10	0.83	0.28	3.57	30,39,45,52	0
4	SO4	A	1345	5/5	0.96	0.15	2.96	25,33,42,46	0
3	XYP	D	1341	10/10	0.90	0.11	2.64	23,25,30,30	0
5	XYS	E	1344	10/10	0.86	0.10	2.37	21,29,34,34	0
3	XYP	A	1341	10/10	0.93	0.10	1.47	20,22,29,30	0
4	SO4	E	1346	5/5	0.82	0.18	1.09	39,40,56,63	0
3	XYP	A	1342	10/10	0.93	0.10	0.93	22,25,32,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NDP	A	1340	48/48	0.96	0.10	0.79	16,20,24,26	0
3	XYP	B	1341	10/10	0.88	0.11	0.54	29,33,36,38	0
2	NDP	E	1340	48/48	0.94	0.11	0.36	18,24,29,33	0
3	XYP	F	1341	10/10	0.86	0.13	0.21	24,28,32,40	0
2	NDP	C	1340	48/48	0.96	0.10	0.18	18,24,26,27	0
2	NDP	B	1340	48/48	0.96	0.09	-0.23	19,23,27,28	0
3	XYP	E	1342	10/10	0.94	0.09	-0.44	19,23,29,30	0
2	NDP	D	1340	48/48	0.96	0.09	-0.44	20,26,30,33	0
3	XYP	C	1342	10/10	0.94	0.08	-0.57	22,25,30,33	0
2	NDP	F	1340	48/48	0.96	0.09	-0.63	19,24,27,29	0
4	SO4	E	1345	5/5	0.98	0.08	-1.24	31,35,40,43	0
5	XYS	B	1342	10/10	0.95	0.06	-1.86	27,30,32,34	0
4	SO4	D	1345	5/5	0.97	0.06	-2.16	33,39,45,45	0
3	XYP	E	1341	10/10	0.88	0.23	-	37,43,50,51	0
3	XYP	D	1342	10/10	0.85	0.25	-	36,41,47,49	0
3	XYP	A	1343	10/10	0.72	0.32	-	37,43,48,51	0
6	DIO	D	1344	6/6	0.91	0.25	-	48,50,54,60	0
4	SO4	E	1347	5/5	0.89	0.34	-	56,57,69,71	0
4	SO4	F	1342	5/5	0.82	0.22	-	45,48,54,62	0
3	XYP	A	1344	10/10	0.79	0.19	-	29,36,42,43	0

6.5 Other polymers

There are no such residues in this entry.