Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2023 – 07:51 PM EDT

PDB ID	:	2AYE
Title	:	Crystal structure of the unliganded E2 DNA Binding Domain from HPV6a
Authors	:	Hooley, E.; Brady, R.L.; Gaston, K.
Deposited on	:	2005-09-07
Resolution	:	2.30 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.30 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.
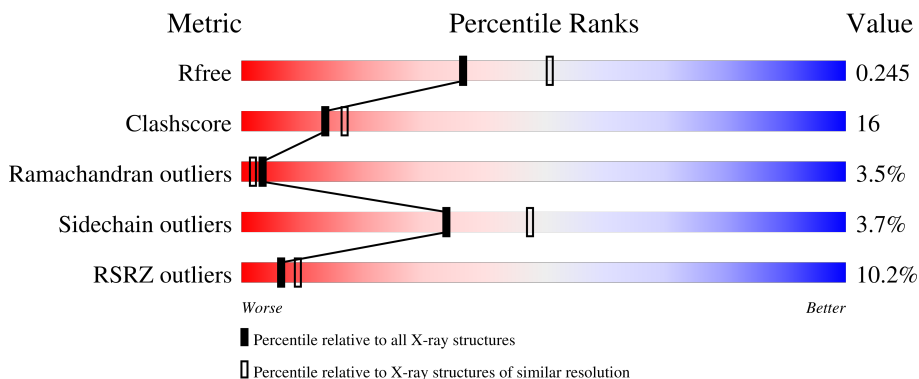
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	87	5% 75% 20% ...
1	B	87	11% 71% 22% 6% .
1	C	87	9% 78% 22%
1	D	87	8% 71% 26% ..
1	E	87	20% 80% 11% 5% .

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Mol	Chain	Length	Quality of chain
1	F	87	8% ▬▬ [====== 70% ======][== 23% ==][5% ••]

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	GOL	D	367	-	-	X	-
3	GOL	F	367	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4571 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 Regulatory protein E2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	86	Total	C	N	O	S	0	1	0
			716	460	133	119	4			
1	B	87	Total	C	N	O	S	0	2	0
			728	467	135	122	4			
1	C	87	Total	C	N	O	S	0	1	0
			722	463	134	121	4			
1	D	87	Total	C	N	O	S	0	1	0
			722	463	134	121	4			
1	E	87	Total	C	N	O	S	0	2	0
			729	468	136	121	4			
1	F	86	Total	C	N	O	S	2	1	0
			716	460	133	119	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	361	MET	LEU	variant	UNP Q84294
B	361	MET	LEU	variant	UNP Q84294
C	361	MET	LEU	variant	UNP Q84294
D	361	MET	LEU	variant	UNP Q84294
E	361	MET	LEU	variant	UNP Q84294
F	361	MET	LEU	variant	UNP Q84294

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

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GOL

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	B	1	Total 6	C 3	O 3	0	0
3	D	1	Total 6	C 3	O 3	0	0
3	F	1	Total 6	C 3	O 3	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total 26	O 26	0	0
4	B	29	Total 29	O 29	0	0
4	C	28	Total 28	O 28	0	0
4	D	27	Total 27	O 27	0	0
4	E	11	Total 11	O 11	0	0
4	F	27	Total 27	O 27	0	0

3 Residue-property plots ⓘ

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: Regulatory protein E2
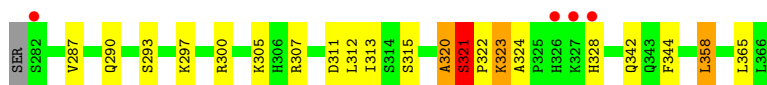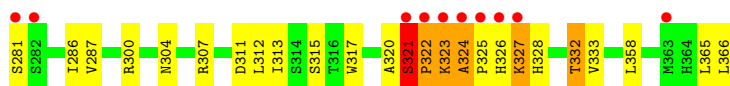
Chain A:

- Molecule 1: Regulatory protein E2

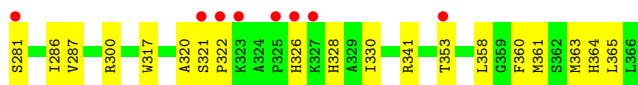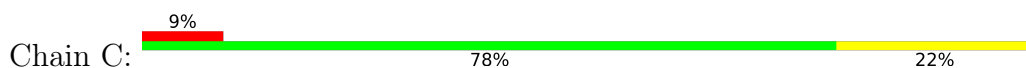Chain B:

- Molecule 1: Regulatory protein E2

Chain C:

- Molecule 1: Regulatory protein E2
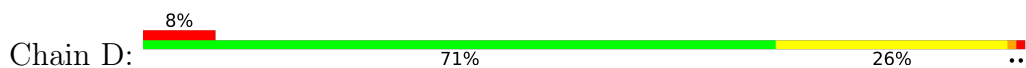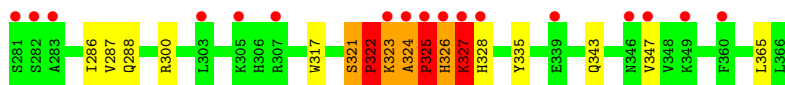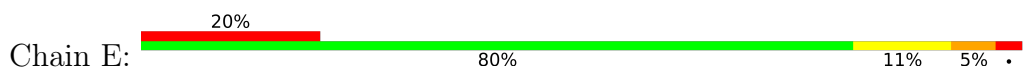
Chain D:

- Molecule 1: Regulatory protein E2

Chain E:

- Molecule 1: Regulatory protein E2

Chain F:

8%

70%　　　　　　　　　　　　　23%　　　　　5%

SER S282 A283 T284 P285 I286 V287 R300 Y301 D311 L312 T316 W317 S321 P322 K323 A324 P325 H326 K327 H328 A329 I330 Q342 N346 K357 L358 G359 F360 M363 H364 L365 L366
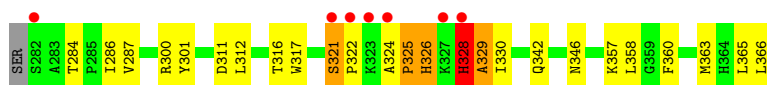
4   Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	97.77Å 106.89Å 74.94Å 90.00° 121.68° 90.00°	Depositor
Resolution (Å)	65.65 – 2.30 16.54 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.0 (65.65-2.30) 97.3 (16.54-2.30)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.80 (at 2.30Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.185 , 0.254 0.180 , 0.245	Depositor DCC
R_{free} test set	1445 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	39.5	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.1	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4571	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.91% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	1.00	0/739	0.91	1/999 (0.1%)
1	B	0.92	0/754	0.97	3/1019 (0.3%)
1	C	0.99	0/745	0.85	0/1007
1	D	0.83	0/745	0.90	2/1007 (0.2%)
1	E	0.82	0/756	0.88	0/1022
1	F	0.91	0/739	0.94	3/999 (0.3%)
All	All	0.92	0/4478	0.91	9/6053 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	1
1	E	0	2
1	F	1	1
All	All	1	5

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	357	LYS	CG-CD-CE	8.71	138.03	111.90
1	B	321	SER	C-N-CD	7.30	143.74	128.40
1	D	321	SER	N-CA-C	7.13	130.26	111.00
1	B	311	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	F	328	HIS	N-CA-C	6.27	127.93	111.00
1	B	311	ASP	CB-CG-OD1	6.17	123.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	321	SER	N-CA-CB	-6.07	101.40	110.50
1	F	329	ALA	N-CA-C	5.55	125.99	111.00
1	A	358	LEU	CA-CB-CG	5.36	127.62	115.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	328	HIS	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	320	ALA	Peptide
1	D	320	ALA	Peptide
1	E	321	SER	Peptide
1	E	325	PRO	Peptide
1	F	328	HIS	Peptide

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	716	0	710	36	0
1	B	728	0	722	33	0
1	C	722	0	715	27	0
1	D	722	0	715	26	0
1	E	729	0	722	17	0
1	F	716	0	710	27	0
2	A	15	0	0	1	0
2	B	5	0	0	0	0
2	C	15	0	0	1	0
2	D	10	0	0	0	0
2	E	5	0	0	1	0
2	F	10	0	0	1	0
3	B	18	0	24	2	0
3	D	6	0	8	5	0
3	F	6	0	8	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	26	0	0	0	0
4	B	29	0	0	3	0
4	C	28	0	0	3	0
4	D	27	0	0	1	1
4	E	11	0	0	0	0
4	F	27	0	0	2	1
All	All	4571	0	4334	136	1

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 16.

All (136) 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:F:321:SER:HB2	1:F:322:PRO:CD	1.68	1.22
1:C:281:SER:HB3	4:C:84:HOH:O	1.49	1.11
1:A:321:SER:HB3	1:A:322:PRO:HD3	1.15	1.10
1:A:321:SER:HB3	1:A:322:PRO:CD	1.85	1.07
1:A:321:SER:CB	1:A:322:PRO:HD3	1.83	1.07
1:D:321:SER:HB2	1:D:322:PRO:HD2	1.30	1.07
1:B:321:SER:O	1:B:323:LYS:N	1.89	1.06
1:A:323:LYS:HD3	1:A:324:ALA:N	1.77	1.00
1:F:321:SER:HB2	1:F:322:PRO:HD3	0.99	0.99
1:F:321:SER:CB	1:F:322:PRO:HD3	1.95	0.94
1:D:321:SER:HB2	1:D:322:PRO:CD	1.97	0.94
1:D:324:ALA:HB3	1:D:325:PRO:HA	1.50	0.94
1:F:321:SER:CB	1:F:322:PRO:CD	2.52	0.86
1:A:323:LYS:HZ1	1:B:313:ILE:H	1.25	0.84
1:A:300:ARG:NH2	2:A:202:SO4:O4	2.10	0.83
1:A:323:LYS:NZ	1:B:313:ILE:H	1.77	0.82
1:D:321:SER:CB	1:D:322:PRO:HD2	2.11	0.81
1:C:287:VAL:HG22	1:C:358:LEU:HD22	1.63	0.80
1:E:324:ALA:HB3	1:E:325:PRO:HD3	1.64	0.79
1:B:321:SER:O	1:B:322:PRO:C	2.18	0.78
1:E:327:LYS:HE2	1:E:328[A]:HIS:NE2	1.99	0.78
1:F:287:VAL:HG22	1:F:358:LEU:HD22	1.65	0.77
1:B:321:SER:HB3	1:B:323:LYS:HG2	1.69	0.74
1:C:300:ARG:HH11	1:C:300:ARG:HG2	1.52	0.74
1:E:325:PRO:HB2	1:E:326:HIS:CD2	2.24	0.73
1:A:323:LYS:HZ2	1:B:312:LEU:HA	1.53	0.72
1:C:321:SER:HB2	1:C:322:PRO:HA	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:LEU:CD1	1:B:286:ILE:HD11	2.20	0.71
1:E:343:GLN:O	1:E:347:VAL:HG23	1.90	0.71
1:E:321:SER:HB2	1:E:322:PRO:O	1.91	0.71
1:A:307:ARG:NH1	1:B:322:PRO:O	2.24	0.70
1:A:342:GLN:HE22	1:C:341:ARG:HH22	1.37	0.69
1:A:313:ILE:HG22	1:B:323:LYS:HD2	1.75	0.68
1:C:326:HIS:HD2	1:C:328:HIS:H	1.40	0.67
1:F:366:LEU:CD2	3:F:367:GOL:H32	2.24	0.67
3:B:368:GOL:O2	4:B:52:HOH:O	1.99	0.67
1:B:321:SER:CB	1:B:323:LYS:HG2	2.24	0.67
1:C:300:ARG:HG2	1:C:300:ARG:NH1	2.10	0.67
1:D:324:ALA:CB	1:D:325:PRO:HA	2.23	0.67
1:E:286:ILE:HD11	1:F:365:LEU:CD1	2.25	0.67
1:A:320:ALA:O	1:A:323:LYS:HD2	1.95	0.66
1:E:325:PRO:HB2	1:E:326:HIS:HD2	1.62	0.65
1:D:324:ALA:CB	1:D:325:PRO:CA	2.74	0.65
1:E:323:LYS:HD2	1:F:311:ASP:OD1	1.97	0.64
1:D:324:ALA:HB3	1:D:325:PRO:CA	2.26	0.63
1:E:286:ILE:HD11	1:F:365:LEU:HD11	1.80	0.63
1:A:321:SER:CB	1:A:322:PRO:CD	2.56	0.63
1:A:287:VAL:HG22	1:A:358:LEU:HD22	1.79	0.62
1:B:321:SER:HB3	1:B:323:LYS:CG	2.25	0.62
1:C:361:MET:CE	3:D:367:GOL:H32	2.29	0.62
1:B:323:LYS:O	1:B:324:ALA:O	2.17	0.62
1:F:366:LEU:HD23	3:F:367:GOL:H32	1.80	0.62
1:C:281:SER:O	1:C:363:MET:CE	2.48	0.62
1:A:320:ALA:O	1:A:323:LYS:CD	2.49	0.60
1:F:328:HIS:N	4:F:148:HOH:O	2.34	0.60
1:C:358:LEU:O	1:D:364:HIS:HE1	1.84	0.60
1:A:293:SER:O	1:A:297:LYS:HG3	2.02	0.59
1:A:323:LYS:HD3	1:A:323:LYS:C	2.23	0.58
1:E:300:ARG:NH2	2:E:203:SO4:O2	2.35	0.58
1:D:343:GLN:O	1:D:347:VAL:HG23	2.04	0.58
1:C:317:TRP:HB3	1:D:317:TRP:HB3	1.86	0.57
1:A:365:LEU:HD13	1:B:286:ILE:HD11	1.86	0.57
1:C:281:SER:O	1:C:363:MET:SD	2.62	0.57
1:A:342:GLN:HE22	1:C:341:ARG:NH2	2.02	0.57
1:C:286:ILE:HD11	1:D:365:LEU:CD1	2.35	0.57
1:A:365:LEU:HD11	1:B:286:ILE:HD11	1.84	0.57
1:A:320:ALA:HB2	1:B:300:ARG:HH21	1.70	0.56
1:C:321:SER:CB	1:C:322:PRO:HA	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:ALA:HB1	4:C:27:HOH:O	2.05	0.56
1:D:321:SER:CB	1:D:322:PRO:CD	2.70	0.56
1:B:366:LEU:HD12	4:B:59:HOH:O	2.06	0.55
1:D:364:HIS:HD2	4:D:73:HOH:O	1.90	0.55
1:F:300:ARG:HH12	1:F:316:THR:CG2	2.20	0.54
1:B:317:TRP:HE1	1:B:332:THR:HG22	1.72	0.54
1:E:287:VAL:HG23	1:E:335:TYR:CE1	2.43	0.54
1:C:361:MET:HE1	3:D:367:GOL:H32	1.90	0.53
1:F:300:ARG:HH12	1:F:316:THR:HG23	1.74	0.53
1:F:366:LEU:HD22	3:F:367:GOL:H32	1.92	0.52
1:C:281:SER:O	1:C:363:MET:HE3	2.09	0.52
1:C:361:MET:HE3	3:D:367:GOL:H32	1.91	0.51
1:D:297:LYS:HG3	1:D:316:THR:HG21	1.91	0.51
1:C:326:HIS:CD2	1:C:328:HIS:H	2.24	0.51
1:B:320:ALA:O	1:B:321:SER:O	2.28	0.51
1:B:287:VAL:HG22	1:B:358:LEU:HD22	1.93	0.50
1:A:321:SER:OG	1:A:322:PRO:HD3	2.08	0.50
1:F:329:ALA:HA	4:F:148:HOH:O	2.11	0.50
1:F:284:THR:O	1:F:360:PHE:HA	2.12	0.50
1:D:345:LEU:HD11	1:D:358:LEU:HD21	1.93	0.49
1:E:321:SER:CB	1:E:322:PRO:O	2.60	0.49
1:E:324:ALA:CB	1:E:325:PRO:HD3	2.39	0.49
1:F:342:GLN:HE21	1:F:346:ASN:ND2	2.11	0.48
1:C:364:HIS:HB3	4:C:132:HOH:O	2.13	0.48
1:B:315:SER:HB2	3:B:369:GOL:H11	1.95	0.47
1:D:281:SER:C	1:D:283:ALA:H	2.18	0.47
1:A:312:LEU:HD22	1:B:324:ALA:HA	1.98	0.46
1:F:342:GLN:HE21	1:F:346:ASN:HD21	1.63	0.46
1:B:365:LEU:O	4:B:59:HOH:O	2.20	0.46
1:D:351:PRO:HB2	1:D:354:ILE:HD12	1.97	0.46
1:C:365:LEU:CD1	1:D:286:ILE:HD11	2.45	0.46
1:E:323:LYS:HB3	1:F:312:LEU:HD23	1.97	0.46
1:F:326:HIS:NE2	1:F:330:ILE:HD11	2.31	0.46
1:E:365:LEU:CD1	1:F:286:ILE:HD11	2.46	0.45
1:D:288:GLN:HG2	1:D:330:ILE:HG23	1.98	0.45
1:D:287:VAL:HG22	1:D:358:LEU:HD22	1.98	0.45
1:A:320:ALA:HB2	1:B:300:ARG:NH2	2.31	0.45
1:A:323:LYS:NZ	1:B:313:ILE:N	2.55	0.45
1:D:283:ALA:HB1	1:D:360:PHE:HB3	1.99	0.45
1:A:311:ASP:O	1:B:323:LYS:HD3	2.16	0.45
1:C:286:ILE:HD11	1:D:365:LEU:HD11	2.00	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:PHE:CD2	1:A:344:PHE:C	2.91	0.44
1:B:304:ASN:O	1:B:307:ARG:HD3	2.17	0.44
1:D:286:ILE:HD12	3:D:367:GOL:H31	1.98	0.44
1:A:320:ALA:N	1:A:323:LYS:HE2	2.32	0.44
1:A:323:LYS:HD3	1:A:324:ALA:H	1.77	0.44
1:C:300:ARG:NH2	2:C:208:SO4:O3	2.51	0.44
1:B:317:TRP:HE1	1:B:332:THR:CG2	2.32	0.43
1:A:358:LEU:HD12	1:C:360:PHE:HZ	1.83	0.43
1:E:365:LEU:HD11	1:F:286:ILE:HD11	2.01	0.43
1:F:324:ALA:HA	1:F:325:PRO:HD3	1.96	0.43
1:B:358:LEU:N	1:B:358:LEU:HD23	2.34	0.43
1:F:316:THR:HG23	2:F:207:SO4:O3	2.18	0.43
1:A:307:ARG:HH12	1:B:322:PRO:HB2	1.84	0.43
1:C:300:ARG:NH1	1:C:300:ARG:CG	2.77	0.43
1:F:329:ALA:HB1	1:F:330:ILE:H	1.67	0.43
1:E:317:TRP:HB3	1:F:317:TRP:HB3	2.01	0.42
1:B:327:LYS:O	1:B:327:LYS:HD3	2.19	0.42
1:D:286:ILE:CD1	3:D:367:GOL:H31	2.49	0.42
1:F:363:MET:HG2	3:F:367:GOL:H31	2.00	0.42
1:C:326:HIS:CE1	1:C:330:ILE:HD11	2.55	0.42
1:A:307:ARG:HE	1:B:323:LYS:NZ	2.18	0.42
1:D:288:GLN:HG2	1:D:330:ILE:CG2	2.50	0.41
1:A:323:LYS:HZ1	1:B:313:ILE:N	2.03	0.40
1:A:323:LYS:O	1:A:324:ALA:C	2.60	0.40
1:A:300:ARG:NH2	1:A:315:SER:HA	2.36	0.40
1:B:313:ILE:HG13	1:B:333:VAL:HG22	2.04	0.40
1:D:287:VAL:HG22	1:D:358:LEU:CD2	2.52	0.40

All (1) 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)
4:D:97:HOH:O	4:F:34:HOH:O[3_455]	2.13	0.07

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	84/87 (97%)	80 (95%)	3 (4%)	1 (1%)	13	14
1	B	86/87 (99%)	78 (91%)	3 (4%)	5 (6%)	1	0
1	C	85/87 (98%)	80 (94%)	5 (6%)	0	100	100
1	D	85/87 (98%)	80 (94%)	2 (2%)	3 (4%)	3	2
1	E	86/87 (99%)	75 (87%)	6 (7%)	5 (6%)	1	0
1	F	84/87 (97%)	74 (88%)	6 (7%)	4 (5%)	2	1
All	All	510/522 (98%)	467 (92%)	25 (5%)	18 (4%)	3	2

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	321	SER
1	B	321	SER
1	B	324	ALA
1	B	325	PRO
1	D	324	ALA
1	E	322	PRO
1	E	324	ALA
1	E	327	LYS
1	F	325	PRO
1	F	328	HIS
1	F	321	SER
1	B	323	LYS
1	D	282	SER
1	E	325	PRO
1	B	322	PRO
1	E	323	LYS
1	F	326	HIS
1	D	321	SER

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	80/81 (99%)	75 (94%)	5 (6%)	18	24
1	B	82/81 (101%)	77 (94%)	5 (6%)	18	25
1	C	81/81 (100%)	80 (99%)	1 (1%)	71	84
1	D	81/81 (100%)	80 (99%)	1 (1%)	71	84
1	E	82/81 (101%)	78 (95%)	4 (5%)	25	35
1	F	80/81 (99%)	78 (98%)	2 (2%)	47	65
All	All	486/486 (100%)	468 (96%)	18 (4%)	34	48

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

Mol	Chain	Res	Type
1	A	290	GLN
1	A	305	LYS
1	A	321	SER
1	A	323	LYS
1	A	328	HIS
1	B	281	SER
1	B	326	HIS
1	B	327	LYS
1	B	328	HIS
1	B	332	THR
1	C	353	THR
1	D	353	THR
1	E	288	GLN
1	E	322	PRO
1	E	326	HIS
1	E	327	LYS
1	F	301	TYR
1	F	328	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	288	GLN
1	A	342	GLN
1	A	343	GLN
1	A	346	ASN
1	B	288	GLN

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Mol	Chain	Res	Type
1	B	346	ASN
1	C	318	HIS
1	C	326	HIS
1	C	342	GLN
1	C	343	GLN
1	C	346	ASN
1	D	346	ASN
1	D	364	HIS
1	E	288	GLN
1	E	326	HIS
1	E	343	GLN
1	E	346	ASN
1	F	328	HIS
1	F	346	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

17 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	SO4	A	206	-	4,4,4	0.20	0	6,6,6	0.27	0
3	GOL	D	367	-	5,5,5	0.89	0	5,5,5	1.77	1 (20%)
2	SO4	C	209	-	4,4,4	0.25	0	6,6,6	1.12	0
3	GOL	B	368	-	5,5,5	0.83	0	5,5,5	1.07	0
2	SO4	F	207	1	4,4,4	0.20	0	6,6,6	0.30	0
2	SO4	A	210	-	4,4,4	0.20	0	6,6,6	0.72	0
2	SO4	F	212	-	4,4,4	0.32	0	6,6,6	1.08	0
2	SO4	C	208	-	4,4,4	0.18	0	6,6,6	1.24	1 (16%)
2	SO4	B	204	-	4,4,4	0.23	0	6,6,6	0.32	0
2	SO4	C	211	-	4,4,4	0.24	0	6,6,6	0.41	0
2	SO4	D	205	-	4,4,4	0.23	0	6,6,6	0.39	0
3	GOL	B	369	-	5,5,5	0.41	0	5,5,5	0.34	0
3	GOL	F	367	-	5,5,5	0.52	0	5,5,5	0.61	0
3	GOL	B	367	-	5,5,5	0.46	0	5,5,5	0.44	0
2	SO4	A	202	-	4,4,4	0.19	0	6,6,6	0.70	0
2	SO4	E	203	-	4,4,4	0.23	0	6,6,6	0.49	0
2	SO4	D	201	1	4,4,4	0.20	0	6,6,6	0.40	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	367	-	-	3/4/4/4	-
3	GOL	B	368	-	-	0/4/4/4	-
3	GOL	B	369	-	-	4/4/4/4	-
3	GOL	F	367	-	-	2/4/4/4	-
3	GOL	B	367	-	-	4/4/4/4	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	367	GOL	O3-C3-C2	3.25	125.77	110.20
2	C	208	SO4	O4-S-O3	2.18	118.36	109.06

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	367	GOL	O1-C1-C2-O2
3	B	367	GOL	C1-C2-C3-O3
3	B	369	GOL	C1-C2-C3-O3
3	D	367	GOL	O1-C1-C2-C3
3	B	367	GOL	O1-C1-C2-C3
3	B	369	GOL	O1-C1-C2-C3
3	F	367	GOL	O1-C1-C2-C3
3	B	367	GOL	O2-C2-C3-O3
3	B	369	GOL	O1-C1-C2-O2
3	B	369	GOL	O2-C2-C3-O3
3	D	367	GOL	O1-C1-C2-O2
3	F	367	GOL	O1-C1-C2-O2
3	D	367	GOL	O2-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	367	GOL	5	0
3	B	368	GOL	1	0
2	F	207	SO4	1	0
2	C	208	SO4	1	0
3	B	369	GOL	1	0
3	F	367	GOL	4	0
2	A	202	SO4	1	0
2	E	203	SO4	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	86/87 (98%)	-0.04	4 (4%)	31	38	11, 20, 32, 34	16 (18%)
1	B	87/87 (100%)	0.57	10 (11%)	4	7	9, 21, 39, 49	22 (25%)
1	C	87/87 (100%)	0.24	8 (9%)	9	12	13, 22, 36, 41	16 (18%)
1	D	87/87 (100%)	0.35	7 (8%)	12	16	18, 28, 38, 53	12 (13%)
1	E	87/87 (100%)	0.97	17 (19%)	1	1	20, 31, 45, 54	17 (19%)
1	F	86/87 (98%)	0.36	7 (8%)	12	16	16, 24, 40, 48	20 (23%)
All	All	520/522 (99%)	0.41	53 (10%)	6	9	9, 25, 40, 54	103 (19%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	324	ALA	26.8
1	B	324	ALA	9.0
1	B	321	SER	8.2
1	B	282	SER	8.1
1	B	326	HIS	7.4
1	F	324	ALA	7.2
1	C	281	SER	6.8
1	B	325	PRO	6.7
1	A	282	SER	6.6
1	E	282	SER	6.6
1	F	323	LYS	6.6
1	B	281	SER	5.7
1	B	323	LYS	5.6
1	E	323	LYS	5.6
1	F	321	SER	5.3
1	F	282	SER	5.3
1	A	327	LYS	4.8
1	E	328[A]	HIS	4.5
1	C	322	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	339	GLU	4.4
1	B	322	PRO	4.4
1	D	324	ALA	4.3
1	C	323	LYS	3.6
1	E	325	PRO	3.6
1	F	328	HIS	3.5
1	B	327	LYS	3.5
1	F	327	LYS	3.5
1	D	352	PRO	3.4
1	D	283	ALA	3.3
1	C	327	LYS	3.3
1	E	281	SER	3.3
1	A	326	HIS	3.1
1	A	328	HIS	3.1
1	D	282	SER	2.9
1	D	308	HIS	2.9
1	F	322	PRO	2.9
1	D	355	ARG	2.8
1	E	307	ARG	2.7
1	C	353	THR	2.7
1	E	283	ALA	2.6
1	E	327	LYS	2.6
1	C	321	SER	2.5
1	E	349	LYS	2.5
1	E	303	LEU	2.5
1	E	346	ASN	2.4
1	C	326	HIS	2.3
1	B	363	MET	2.3
1	C	325	PRO	2.3
1	E	326	HIS	2.2
1	E	305	LYS	2.1
1	E	347	VAL	2.1
1	E	360	PHE	2.1
1	D	281	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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(Å^2)	Q<0.9
3	GOL	B	368	6/6	0.80	0.24	26,44,48,52	0
3	GOL	B	369	6/6	0.81	0.23	29,40,44,49	0
2	SO4	A	206	5/5	0.84	0.40	86,87,87,88	0
3	GOL	D	367	6/6	0.87	0.16	26,34,38,38	0
2	SO4	F	207	5/5	0.89	0.24	76,77,79,79	0
2	SO4	D	201	5/5	0.89	0.24	61,64,65,67	0
3	GOL	F	367	6/6	0.89	0.20	41,46,47,48	0
3	GOL	B	367	6/6	0.90	0.14	41,45,48,49	0
2	SO4	C	208	5/5	0.92	0.17	34,38,39,41	5
2	SO4	E	203	5/5	0.93	0.22	58,58,61,63	0
2	SO4	C	209	5/5	0.95	0.10	32,34,39,39	5
2	SO4	F	212	5/5	0.96	0.20	31,32,36,37	5
2	SO4	D	205	5/5	0.98	0.18	57,59,59,60	0
2	SO4	C	211	5/5	0.98	0.12	28,28,28,33	5
2	SO4	A	202	5/5	0.98	0.14	42,42,45,46	0
2	SO4	B	204	5/5	0.99	0.17	41,45,47,48	0
2	SO4	A	210	5/5	0.99	0.12	24,25,28,28	5

6.5 Other polymers (i)

There are no such residues in this entry.