



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:51 pm BST

PDB ID : 4JAX
Title : Crystal structure of dimeric KIHxk1 in crystal form X
Authors : Kuettner, E.B.; Strater, N.; Kettner, K.; Otto, A.; Lilie, H.; Golbik, R.P.;
Kriegel, T.M.
Deposited on : 2013-02-19
Resolution : 2.26 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.11
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) : 2.11

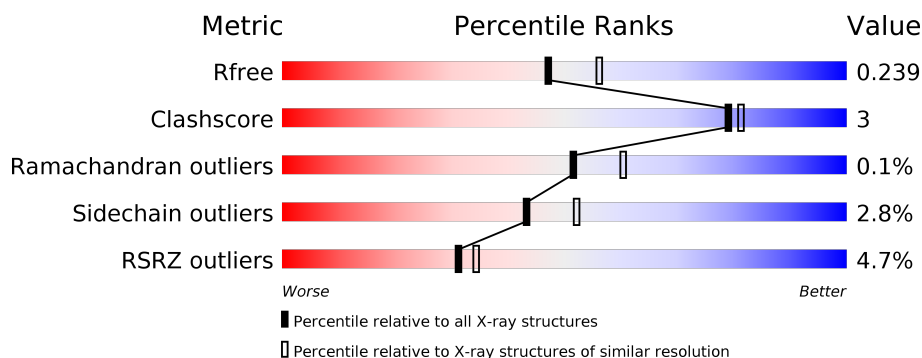
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.26 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	485	<div> <div>0%</div> <div>89% 7% ..</div> </div>
1	B	485	<div> <div>3%</div> <div>89% 8% ..</div> </div>
1	C	485	<div> <div>3%</div> <div>90% 7% ..</div> </div>
1	D	485	<div> <div>3%</div> <div>90% 7% .</div> </div>
1	E	485	<div> <div>5%</div> <div>91% 6% .</div> </div>
1	F	485	<div> <div>13%</div> <div>82% 11% . 5%</div> </div>

2 Entry composition [i](#)

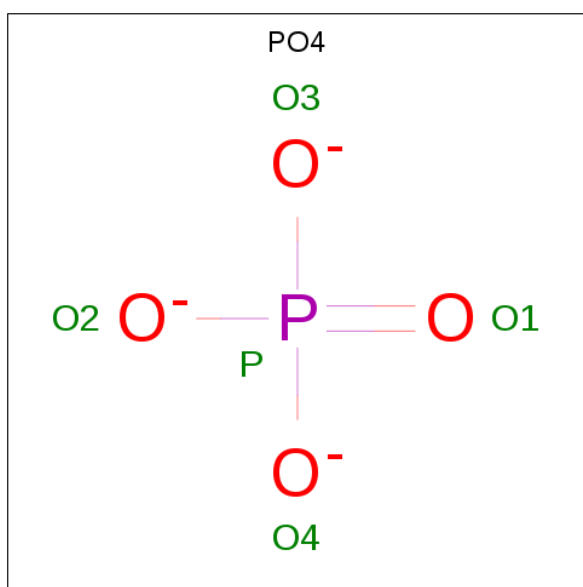
There are 4 unique types of molecules in this entry. The entry contains 22473 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Hexokinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	P	S	0	1	0
			3664	2330	603	714	1	16			
1	B	472	Total	C	N	O	P	S	0	2	0
			3681	2340	606	718	1	16			
1	C	475	Total	C	N	O	P	S	0	0	0
			3698	2349	610	722	1	16			
1	D	473	Total	C	N	O	P	S	0	0	0
			3682	2340	605	720	1	16			
1	E	471	Total	C	N	O	P	S	0	0	0
			3669	2332	602	718	1	16			
1	F	460	Total	C	N	O	P	S	0	0	0
			3592	2287	586	702	1	16			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	110	Total	O	0	0
			110	110		
4	B	55	Total	O	0	0
			55	55		
4	C	72	Total	O	0	0
			72	72		
4	D	47	Total	O	0	0
			47	47		

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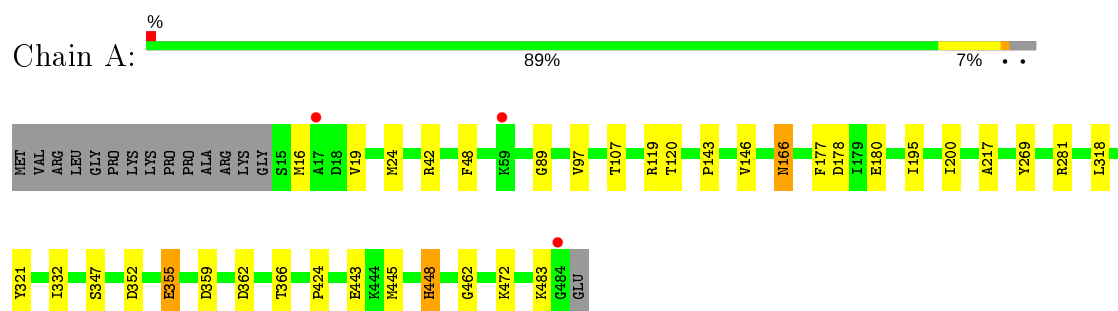
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	36	Total	O	0	0
			36	36		
4	F	34	Total	O	0	0
			34	34		

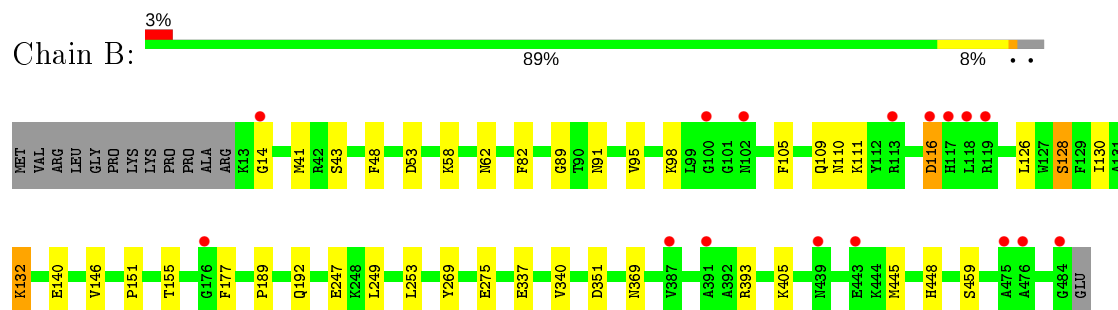
3 Residue-property plots [i](#)

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.

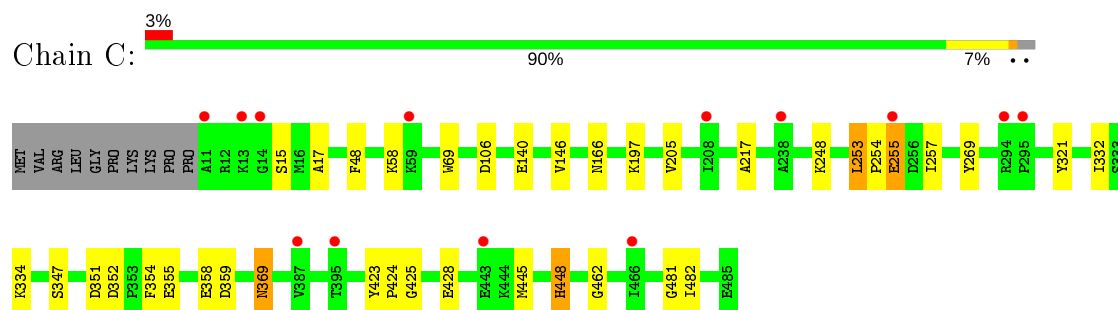
• Molecule 1: Hexokinase



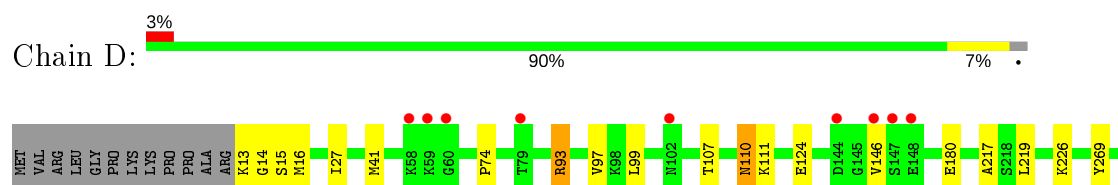
• Molecule 1: Hexokinase

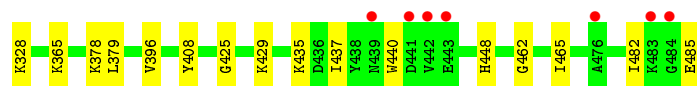


• Molecule 1: Hexokinase

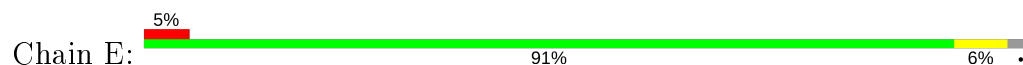


• Molecule 1: Hexokinase

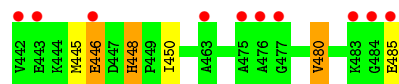
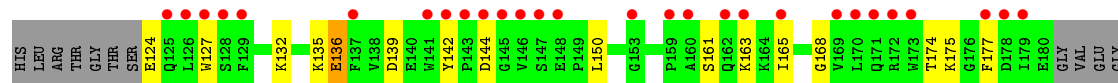
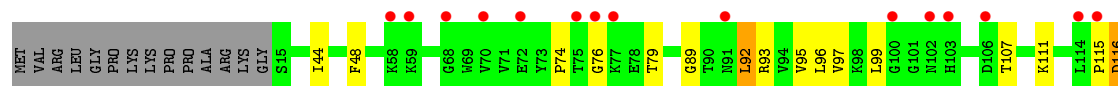
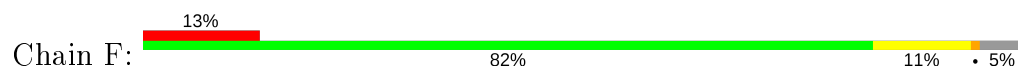




• Molecule 1: Hexokinase



• Molecule 1: Hexokinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.81Å 178.30Å 216.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.60 – 2.26 29.58 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.60-2.26) 99.9 (29.58-2.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.80 (at 2.26Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.200 , 0.240 0.199 , 0.239	Depositor DCC
R_{free} test set	1911 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22473	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4, SEP

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	0.55	0/3733	0.72	3/5057 (0.1%)
1	B	0.52	0/3754	0.68	0/5082
1	C	0.51	0/3760	0.67	0/5088
1	D	0.48	0/3744	0.67	2/5067 (0.0%)
1	E	0.46	0/3732	0.62	0/5054
1	F	0.51	0/3652	0.66	0/4943
All	All	0.51	0/22375	0.67	5/30291 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	93	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	A	42	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	A	281	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	281	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	D	365	LYS	CD-CE-NZ	5.01	123.23	111.70

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	3664	0	3644	18	0
1	B	3681	0	3659	20	0
1	C	3698	0	3679	24	0
1	D	3682	0	3661	21	0
1	E	3669	0	3647	15	0
1	F	3592	0	3571	32	0
2	A	20	0	0	0	0
2	B	5	0	0	0	0
2	C	20	0	0	0	0
2	D	20	0	0	0	0
2	E	15	0	0	1	0
2	F	5	0	0	0	0
3	A	12	0	16	0	0
3	B	6	0	8	0	0
3	C	12	0	16	0	0
3	D	6	0	8	1	0
3	E	12	0	16	1	0
4	A	110	0	0	1	0
4	B	55	0	0	0	0
4	C	72	0	0	1	0
4	D	47	0	0	0	0
4	E	36	0	0	0	0
4	F	34	0	0	1	0
All	All	22473	0	21925	125	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 3.

All (125) 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:D:14:GLY:O	1:D:15:SEP:HB3	1.59	0.98
1:F:97:VAL:HG22	1:F:107:THR:HG22	1.55	0.87
1:C:253:LEU:HD13	1:C:254:PRO:HD2	1.58	0.83
1:A:166:ASN:H	1:A:166:ASN:HD22	1.29	0.78
1:F:127:TRP:HB2	1:F:194:GLN:HG3	1.69	0.73
1:B:189:PRO:HA	1:B:192:GLN:HE21	1.52	0.72
1:A:355:GLU:HG2	1:D:110:ASN:OD1	1.91	0.70
1:C:334:LYS:HZ2	1:C:369:ASN:HB2	1.59	0.68
1:C:253:LEU:HD11	1:C:257:ILE:HB	1.76	0.67
1:D:16:MET:HE3	1:D:27:ILE:HD13	1.76	0.66
1:B:116:ASP:OD2	1:B:116:ASP:N	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:115:PRO:O	1:F:116:ASP:HB3	1.94	0.65
1:D:110:ASN:HD22	1:D:111:LYS:H	1.45	0.65
1:D:217:ALA:HB2	1:D:462:GLY:HA2	1.81	0.63
1:C:334:LYS:NZ	1:C:369:ASN:HB2	2.14	0.62
1:C:352:ASP:CG	1:C:359:ASP:HB2	2.22	0.60
1:E:110:ASN:HD22	1:E:111:LYS:H	1.50	0.59
1:A:97:VAL:HG22	1:A:107:THR:HG22	1.85	0.59
1:E:41:MET:HE2	1:E:437:ILE:HD11	1.83	0.59
1:A:89:GLY:HA2	1:A:177:PHE:HE1	1.68	0.59
1:B:89:GLY:HA2	1:B:177:PHE:HE1	1.68	0.59
1:D:41:MET:HE2	1:D:437:ILE:HD11	1.84	0.59
1:C:253:LEU:CD1	1:C:257:ILE:HB	2.33	0.59
1:B:58:LYS:HG3	1:B:247:GLU:HG2	1.86	0.58
1:B:62:ASN:ND2	1:B:275:GLU:OE2	2.38	0.57
1:F:219:LEU:HA	1:F:225:THR:HB	1.87	0.57
1:E:233:THR:HG23	2:E:501:PO4:O3	2.05	0.56
1:D:217:ALA:HB2	1:D:462:GLY:CA	2.36	0.55
1:B:111:LYS:HB2	1:C:354:PHE:CE2	2.42	0.55
1:F:298:GLN:HB2	1:F:301:GLU:HB3	1.89	0.55
1:F:44:ILE:O	1:F:48:PHE:HB2	2.08	0.54
1:B:95:VAL:HG13	1:B:109:GLN:HB3	1.90	0.53
1:D:74:PRO:HD2	1:D:219:LEU:HD23	1.89	0.53
1:F:297:GLN:O	1:F:298:GLN:HG2	2.08	0.53
1:C:321:TYR:CE2	1:C:332:ILE:HG12	2.45	0.53
1:F:89:GLY:HA2	1:F:177:PHE:CE1	2.45	0.52
1:F:445:MET:HA	1:F:448:HIS:CE1	2.45	0.52
1:C:347:SER:O	1:C:424:PRO:HG2	2.10	0.51
1:D:97:VAL:HG22	1:D:107:THR:HG22	1.92	0.51
1:C:253:LEU:HD13	1:C:254:PRO:CD	2.36	0.51
1:E:148:GLU:HB2	1:E:149:PRO:HD2	1.92	0.51
1:E:58:LYS:HG3	1:E:247:GLU:HG2	1.92	0.51
1:A:143:PRO:HG3	1:D:13:LYS:HD2	1.92	0.51
1:E:234:GLY:HA3	3:E:504:GOL:H31	1.94	0.50
1:F:89:GLY:HA2	1:F:177:PHE:HE1	1.76	0.50
1:F:93:ARG:HG2	1:F:111:LYS:HG3	1.93	0.50
1:F:135:LYS:HD2	1:F:198:LEU:HD12	1.93	0.50
1:E:74:PRO:HD2	1:E:219:LEU:HD23	1.93	0.50
1:F:132:LYS:O	1:F:136:GLU:HG2	2.11	0.50
1:E:394:LEU:O	1:E:397:CYS:HB2	2.12	0.49
1:F:92:LEU:C	1:F:92:LEU:HD12	2.33	0.49
1:B:337[B]:GLU:HB3	1:B:340:VAL:HB	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:192:GLN:O	1:F:196:GLU:HG2	2.13	0.49
1:C:347:SER:HB2	1:C:424:PRO:HD3	1.95	0.49
1:F:79:THR:HA	1:F:99:LEU:O	2.13	0.48
1:D:110:ASN:ND2	1:D:111:LYS:H	2.10	0.48
1:C:448:HIS:HD2	4:C:608:HOH:O	1.96	0.47
1:B:155:THR:HG21	1:B:459:SER:HB2	1.96	0.47
1:F:76:GLY:HA2	1:F:220:TYR:CE1	2.49	0.47
1:C:347:SER:O	1:C:351:ASP:HB2	2.15	0.47
1:F:168:GLY:HA3	1:F:207:LEU:HD13	1.96	0.47
1:B:82:PHE:CD1	1:B:151:PRO:HG2	2.50	0.46
1:C:166:ASN:HB3	1:C:205:VAL:O	2.16	0.46
1:A:166:ASN:N	1:A:166:ASN:HD22	2.05	0.46
1:B:53:ASP:OD1	1:B:405:LYS:HE2	2.15	0.46
1:D:328:LYS:HB3	3:D:505:GOL:O3	2.15	0.46
1:D:41:MET:CE	1:D:437:ILE:HD11	2.46	0.46
1:B:110:ASN:OD1	1:C:355:GLU:HB2	2.16	0.46
1:F:394:LEU:O	1:F:397:CYS:HB2	2.16	0.46
1:D:226:LYS:HD3	1:D:408:TYR:CG	2.51	0.45
1:A:321:TYR:CZ	1:A:332:ILE:HG12	2.52	0.45
1:F:188:VAL:HB	1:F:189:PRO:HD3	1.98	0.45
1:F:165:ILE:HG22	1:F:480:VAL:HB	1.98	0.45
1:D:379:LEU:C	1:D:379:LEU:HD23	2.37	0.45
1:A:119:ARG:HG3	4:A:659:HOH:O	2.17	0.45
1:A:120:THR:HG22	1:A:178:ASP:HB3	1.98	0.45
1:E:363:LEU:O	1:E:367:ASN:HB2	2.17	0.45
1:F:230:ILE:C	1:F:231:ILE:HG13	2.36	0.44
1:A:19:VAL:HB	1:A:24:MET:HE1	1.98	0.44
1:C:217:ALA:HB2	1:C:462:GLY:HA2	2.00	0.44
1:E:217:ALA:HB2	1:E:462:GLY:HA2	1.99	0.44
1:D:425:GLY:O	1:D:429:LYS:HG3	2.17	0.44
1:C:255:GLU:H	1:C:255:GLU:HG2	1.54	0.44
1:A:445:MET:HA	1:A:448:HIS:CE1	2.53	0.43
1:A:217:ALA:HB2	1:A:462:GLY:HA2	2.00	0.43
1:C:15:SEP:O1P	1:C:17:ALA:HB2	2.17	0.43
1:F:74:PRO:HG3	1:F:216:VAL:HG13	2.00	0.43
1:E:46:LYS:HA	1:E:46:LYS:HD3	1.60	0.43
1:B:445:MET:HA	1:B:448:HIS:CD2	2.54	0.43
1:C:425:GLY:HA2	1:C:428:GLU:OE1	2.19	0.42
1:E:41:MET:CE	1:E:437:ILE:HD11	2.47	0.42
1:F:298:GLN:HE21	1:F:298:GLN:HB3	1.53	0.42
1:B:249:LEU:HD13	1:B:253:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ASP:CG	1:A:359:ASP:HB2	2.40	0.42
1:C:423:TYR:HA	1:C:424:PRO:HD3	1.86	0.42
1:A:166:ASN:ND2	1:A:166:ASN:H	2.08	0.42
1:B:14:GLY:HA2	1:C:140:GLU:HG3	2.02	0.42
1:F:271:SER:HA	1:F:298:GLN:HA	2.02	0.42
1:C:69:TRP:CE3	1:C:481:GLY:HA2	2.54	0.42
1:E:358:GLU:HG2	1:E:358:GLU:H	1.57	0.42
1:F:142:TYR:CE1	1:F:150:LEU:HD11	2.55	0.42
1:F:281:ARG:HD2	4:F:615:HOH:O	2.19	0.42
1:D:482:ILE:HG13	1:D:485:GLU:HG2	2.02	0.41
1:F:163:LYS:HB3	1:F:485:GLU:HG3	2.00	0.41
1:A:195:ILE:HG23	1:A:200:ILE:HB	2.02	0.41
1:B:41:MET:CE	1:B:393:ARG:O	2.68	0.41
1:F:174:THR:O	1:F:175:LYS:HB2	2.20	0.41
1:F:440:TRP:HH2	1:F:450:ILE:HB	1.84	0.41
1:A:19:VAL:HB	1:A:24:MET:CE	2.50	0.41
1:B:98:LYS:O	1:B:105:PHE:HA	2.21	0.41
1:F:446:GLU:HG3	1:F:446:GLU:H	1.61	0.41
1:A:347:SER:O	1:A:424:PRO:HG2	2.20	0.41
1:B:41:MET:HE3	1:B:393:ARG:O	2.20	0.41
1:D:99:LEU:HD21	1:D:465:ILE:HG12	2.03	0.41
1:D:16:MET:CE	1:D:27:ILE:HD13	2.49	0.41
1:E:77:LYS:O	1:E:101:GLY:HA2	2.21	0.41
1:B:126:LEU:O	1:B:130:ILE:HG13	2.20	0.40
1:C:445:MET:HA	1:C:448:HIS:CE1	2.56	0.40
1:F:96:LEU:O	1:F:107:THR:HA	2.21	0.40
1:E:379:LEU:C	1:E:379:LEU:HD23	2.41	0.40
1:B:128:SER:O	1:B:132:LYS:HB2	2.22	0.40
1:C:58:LYS:HG2	1:C:248:LYS:HA	2.04	0.40
1:D:15:SEP:HB2	1:D:16:MET:H	1.68	0.40
1:D:435:LYS:HA	1:D:440:TRP:CE3	2.56	0.40
1:A:362:ASP:O	1:A:366:THR:HB	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	469/485 (97%)	450 (96%)	18 (4%)	1 (0%)	47	55
1	B	471/485 (97%)	450 (96%)	21 (4%)	0	100	100
1	C	472/485 (97%)	454 (96%)	18 (4%)	0	100	100
1	D	470/485 (97%)	447 (95%)	23 (5%)	0	100	100
1	E	469/485 (97%)	450 (96%)	19 (4%)	0	100	100
1	F	454/485 (94%)	428 (94%)	25 (6%)	1 (0%)	47	55
All	All	2805/2910 (96%)	2679 (96%)	124 (4%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	MET
1	F	201	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	400/411 (97%)	389 (97%)	11 (3%)	43	52
1	B	402/411 (98%)	391 (97%)	11 (3%)	44	54
1	C	402/411 (98%)	391 (97%)	11 (3%)	44	54
1	D	401/411 (98%)	392 (98%)	9 (2%)	52	61
1	E	400/411 (97%)	389 (97%)	11 (3%)	43	52
1	F	392/411 (95%)	378 (96%)	14 (4%)	35	42
All	All	2397/2466 (97%)	2330 (97%)	67 (3%)	43	52

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	PHE
1	A	146	VAL
1	A	166	ASN
1	A	180	GLU
1	A	269	TYR
1	A	318	LEU
1	A	355	GLU
1	A	443	GLU
1	A	448	HIS
1	A	472	LYS
1	A	483	LYS
1	B	43	SER
1	B	48	PHE
1	B	91	ASN
1	B	116	ASP
1	B	128	SER
1	B	132	LYS
1	B	140	GLU
1	B	146	VAL
1	B	269	TYR
1	B	351	ASP
1	B	369	ASN
1	C	48	PHE
1	C	106	ASP
1	C	146	VAL
1	C	197	LYS
1	C	253	LEU
1	C	255	GLU
1	C	269	TYR
1	C	358	GLU
1	C	369	ASN
1	C	448	HIS
1	C	482	ILE
1	D	93	ARG
1	D	110	ASN
1	D	124	GLU
1	D	146	VAL
1	D	180	GLU
1	D	269	TYR
1	D	378	LYS
1	D	396	VAL
1	D	448	HIS
1	E	18	ASP

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Mol	Chain	Res	Type
1	E	22	ASN
1	E	27	ILE
1	E	106	ASP
1	E	110	ASN
1	E	154	PHE
1	E	250	GLU
1	E	269	TYR
1	E	347	SER
1	E	351	ASP
1	E	358	GLU
1	F	92	LEU
1	F	95	VAL
1	F	116	ASP
1	F	124	GLU
1	F	136	GLU
1	F	139	ASP
1	F	144	ASP
1	F	161	SER
1	F	269	TYR
1	F	298	GLN
1	F	333	SER
1	F	446	GLU
1	F	448	HIS
1	F	480	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	166	ASN
1	A	448	HIS
1	B	192	GLN
1	C	102	ASN
1	C	367	ASN
1	C	369	ASN
1	C	448	HIS
1	D	62	ASN
1	D	110	ASN
1	D	367	ASN
1	D	471	GLN
1	E	22	ASN
1	E	102	ASN

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Mol	Chain	Res	Type
1	E	110	ASN
1	F	110	ASN
1	F	125	GLN
1	F	194	GLN
1	F	298	GLN
1	F	367	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	$\# Z > 2$
1	SEP	C	15	1	8,9,10	0.64	0	8,12,14	1.25	0
1	SEP	A	15	1	8,9,10	0.55	0	8,12,14	1.71	2 (25%)
1	SEP	F	15	1	8,9,10	0.65	0	8,12,14	1.99	3 (37%)
1	SEP	D	15	1	8,9,10	0.59	0	8,12,14	2.31	1 (12%)
1	SEP	E	15	1	8,9,10	0.65	0	8,12,14	1.44	1 (12%)
1	SEP	B	15	1	8,9,10	0.73	0	8,12,14	3.73	4 (50%)

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
1	SEP	C	15	1	-	2/5/8/10	-
1	SEP	A	15	1	-	3/5/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	F	15	1	-	1/5/8/10	-
1	SEP	D	15	1	-	5/5/8/10	-
1	SEP	E	15	1	-	5/5/8/10	-
1	SEP	B	15	1	-	1/5/8/10	-

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	15	SEP	OG-CB-CA	8.96	116.87	108.14
1	D	15	SEP	OG-CB-CA	6.04	114.02	108.14
1	B	15	SEP	O2P-P-OG	-4.19	95.57	106.73
1	F	15	SEP	OG-CB-CA	3.88	111.92	108.14
1	A	15	SEP	OG-CB-CA	2.91	110.98	108.14
1	E	15	SEP	OG-CB-CA	2.69	110.76	108.14
1	B	15	SEP	OG-P-O1P	2.57	113.69	106.47
1	A	15	SEP	O2P-P-OG	-2.46	100.17	106.73
1	F	15	SEP	O3P-P-OG	-2.30	100.62	106.73
1	F	15	SEP	O3P-P-O2P	2.26	116.26	107.64
1	B	15	SEP	O3P-P-O2P	2.12	115.74	107.64

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	15	SEP	CA-CB-OG-P
1	A	15	SEP	CB-OG-P-O1P
1	F	15	SEP	N-CA-CB-OG
1	D	15	SEP	N-CA-CB-OG
1	D	15	SEP	CA-CB-OG-P
1	D	15	SEP	CB-OG-P-O1P
1	D	15	SEP	CB-OG-P-O2P
1	E	15	SEP	CA-CB-OG-P
1	E	15	SEP	CB-OG-P-O1P
1	E	15	SEP	CB-OG-P-O3P
1	B	15	SEP	N-CA-CB-OG
1	C	15	SEP	N-CA-CB-OG
1	A	15	SEP	N-CA-CB-OG
1	E	15	SEP	N-CA-CB-OG
1	A	15	SEP	CB-OG-P-O3P
1	D	15	SEP	CB-OG-P-O3P

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Mol	Chain	Res	Type	Atoms
1	E	15	SEP	CB-OG-P-O2P

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	15	SEP	1	0
1	D	15	SEP	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

25 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	PO4	E	501	-	4,4,4	0.92	0	6,6,6	0.82	0
2	PO4	B	501	-	4,4,4	0.91	0	6,6,6	1.38	1 (16%)
2	PO4	D	502	-	4,4,4	0.94	0	6,6,6	0.69	0
2	PO4	A	504	-	4,4,4	0.82	0	6,6,6	0.51	0
2	PO4	C	504	-	4,4,4	0.70	0	6,6,6	0.66	0
2	PO4	A	503	-	4,4,4	0.95	0	6,6,6	0.85	0
3	GOL	D	505	-	5,5,5	0.51	0	5,5,5	0.41	0
3	GOL	E	505	-	5,5,5	0.39	0	5,5,5	0.47	0
3	GOL	C	506	-	5,5,5	0.46	0	5,5,5	0.40	0
2	PO4	E	502	-	4,4,4	0.80	0	6,6,6	1.05	0
2	PO4	C	502	-	4,4,4	0.78	0	6,6,6	0.41	0
2	PO4	F	501	-	4,4,4	0.85	0	6,6,6	0.71	0
2	PO4	C	501	-	4,4,4	0.83	0	6,6,6	0.52	0
3	GOL	E	504	-	5,5,5	0.36	0	5,5,5	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	506	-	5,5,5	0.53	0	5,5,5	0.52	0
2	PO4	A	501	-	4,4,4	0.82	0	6,6,6	0.51	0
2	PO4	D	501	-	4,4,4	0.88	0	6,6,6	0.48	0
2	PO4	C	503	-	4,4,4	0.72	0	6,6,6	0.77	0
3	GOL	B	502	-	5,5,5	0.22	0	5,5,5	1.12	0
2	PO4	D	503	-	4,4,4	0.88	0	6,6,6	0.53	0
2	PO4	A	502	-	4,4,4	0.98	0	6,6,6	1.27	1 (16%)
2	PO4	E	503	-	4,4,4	0.91	0	6,6,6	0.48	0
2	PO4	D	504	-	4,4,4	0.79	0	6,6,6	0.52	0
3	GOL	C	505	-	5,5,5	0.45	0	5,5,5	0.83	0
3	GOL	A	505	-	5,5,5	0.43	0	5,5,5	1.11	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	C	506	-	-	2/4/4/4	-
3	GOL	E	504	-	-	4/4/4/4	-
3	GOL	B	502	-	-	4/4/4/4	-
3	GOL	C	505	-	-	2/4/4/4	-
3	GOL	A	505	-	-	4/4/4/4	-
3	GOL	D	505	-	-	2/4/4/4	-
3	GOL	A	506	-	-	2/4/4/4	-
3	GOL	E	505	-	-	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(°)	Ideal(°)
2	B	501	PO4	O4-P-O2	2.41	115.71	107.97
2	A	502	PO4	O3-P-O2	2.32	115.43	107.97

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	505	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	E	505	GOL	O2-C2-C3-O3
3	E	504	GOL	C1-C2-C3-O3
3	B	502	GOL	O1-C1-C2-C3
3	A	505	GOL	O1-C1-C2-C3
3	E	505	GOL	O1-C1-C2-C3
3	C	506	GOL	O1-C1-C2-C3
3	A	506	GOL	C1-C2-C3-O3
3	B	502	GOL	C1-C2-C3-O3
3	A	505	GOL	C1-C2-C3-O3
3	C	506	GOL	O1-C1-C2-O2
3	E	504	GOL	O2-C2-C3-O3
3	A	506	GOL	O2-C2-C3-O3
3	B	502	GOL	O2-C2-C3-O3
3	A	505	GOL	O1-C1-C2-O2
3	A	505	GOL	O2-C2-C3-O3
3	E	504	GOL	O1-C1-C2-O2
3	B	502	GOL	O1-C1-C2-O2
3	C	505	GOL	O2-C2-C3-O3
3	C	505	GOL	C1-C2-C3-O3
3	E	505	GOL	O1-C1-C2-O2
3	D	505	GOL	O1-C1-C2-C3
3	D	505	GOL	C1-C2-C3-O3
3	E	504	GOL	O1-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	501	PO4	1	0
3	D	505	GOL	1	0
3	E	504	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	469/485 (96%)	-0.37	3 (0%) 89 89	23, 34, 56, 81	0
1	B	471/485 (97%)	-0.11	16 (3%) 45 47	27, 41, 74, 102	0
1	C	474/485 (97%)	-0.05	13 (2%) 54 57	19, 42, 80, 98	0
1	D	472/485 (97%)	-0.13	16 (3%) 45 47	25, 46, 74, 105	0
1	E	470/485 (96%)	0.09	22 (4%) 31 34	23, 52, 97, 156	0
1	F	459/485 (94%)	0.57	63 (13%) 3 2	25, 59, 115, 146	0
All	All	2815/2910 (96%)	-0.00	133 (4%) 31 34	19, 44, 92, 156	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	143	PRO	8.2
1	F	144	ASP	7.7
1	F	165	ILE	7.5
1	F	179	ILE	7.3
1	E	329	ASP	7.0
1	F	146	VAL	5.9
1	F	477	GLY	5.9
1	F	147	SER	5.8
1	F	475	ALA	5.7
1	F	177	PHE	5.6
1	F	476	ALA	5.2
1	F	170	LEU	5.1
1	F	159	PRO	5.0
1	F	173	TRP	5.0
1	F	126	LEU	4.8
1	F	484	GLY	4.8
1	F	128	SER	4.7
1	D	443	GLU	4.5
1	F	172	ARG	4.5

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Mol	Chain	Res	Type	RSRZ
1	F	251	GLY	4.4
1	F	145	GLY	4.2
1	F	141	TRP	4.1
1	F	255	GLU	4.0
1	F	114	LEU	4.0
1	F	142	TYR	3.9
1	E	16	MET	3.9
1	D	148	GLU	3.9
1	E	17	ALA	3.8
1	F	59	LYS	3.8
1	C	11	ALA	3.7
1	D	59	LYS	3.7
1	D	147	SER	3.4
1	D	144	ASP	3.4
1	F	260	ASP	3.4
1	E	59	LYS	3.3
1	E	443	GLU	3.2
1	D	58	LYS	3.2
1	F	178	ASP	3.2
1	E	21	ALA	3.2
1	F	163	LYS	3.2
1	F	76	GLY	3.2
1	F	442	VAL	3.1
1	F	446	GLU	3.1
1	F	187	VAL	3.1
1	F	171	GLN	3.0
1	B	14	GLY	3.0
1	B	176	GLY	3.0
1	F	75	THR	3.0
1	F	441	ASP	3.0
1	F	58	LYS	3.0
1	C	294	ARG	2.9
1	F	169	VAL	2.9
1	F	153	GLY	2.8
1	E	439	ASN	2.8
1	A	484	GLY	2.8
1	B	100	GLY	2.8
1	B	117	HIS	2.8
1	F	77	LYS	2.8
1	E	60	GLY	2.7
1	B	387	VAL	2.6
1	D	476	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	483	LYS	2.6
1	F	103	HIS	2.6
1	E	20	PRO	2.6
1	E	444	LYS	2.6
1	E	22	ASN	2.6
1	F	409	LYS	2.6
1	C	387	VAL	2.5
1	E	25	GLU	2.5
1	E	441	ASP	2.5
1	F	148	GLU	2.5
1	F	247	GLU	2.5
1	E	325	PHE	2.5
1	F	137	PHE	2.5
1	D	442	VAL	2.5
1	D	79	THR	2.5
1	F	443	GLU	2.4
1	D	483	LYS	2.4
1	A	17	ALA	2.4
1	C	295	PRO	2.4
1	F	106	ASP	2.4
1	F	102	ASN	2.4
1	D	146	VAL	2.4
1	B	439	ASN	2.4
1	B	476	ALA	2.4
1	E	18	ASP	2.4
1	F	259	PRO	2.4
1	C	466	ILE	2.4
1	E	208	ILE	2.4
1	E	19	VAL	2.4
1	B	116	ASP	2.3
1	B	391	ALA	2.3
1	B	443	GLU	2.3
1	B	119	ARG	2.3
1	F	70	VAL	2.3
1	B	113	ARG	2.3
1	D	441	ASP	2.3
1	F	72	GLU	2.3
1	F	127	TRP	2.3
1	F	238	ALA	2.3
1	F	125	GLN	2.3
1	F	160	ALA	2.3
1	B	118	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	162	GLN	2.2
1	F	115	PRO	2.2
1	F	129	PHE	2.2
1	F	485	GLU	2.2
1	C	59	LYS	2.2
1	B	484	GLY	2.2
1	C	14	GLY	2.2
1	D	484	GLY	2.2
1	C	255	GLU	2.2
1	E	294	ARG	2.2
1	D	60	GLY	2.2
1	F	91	ASN	2.2
1	E	366	THR	2.2
1	C	13	LYS	2.2
1	E	58	LYS	2.2
1	F	196	GLU	2.2
1	C	443	GLU	2.2
1	B	102	ASN	2.1
1	F	100	GLY	2.2
1	E	399	VAL	2.1
1	C	208	ILE	2.1
1	D	439	ASN	2.1
1	F	463	ALA	2.1
1	E	368	LEU	2.0
1	F	68	GLY	2.0
1	C	395	THR	2.0
1	D	102	ASN	2.0
1	A	59	LYS	2.0
1	B	475	ALA	2.0
1	C	238	ALA	2.0

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

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
1	SEP	C	15	10/11	0.82	0.28	83,95,111,115	0
1	SEP	B	15	10/11	0.83	0.15	68,81,87,91	0
1	SEP	E	15	10/11	0.84	0.30	103,126,142,144	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	SEP	A	15	10/11	0.91	0.13	69,85,92,97	0
1	SEP	F	15	10/11	0.91	0.12	69,75,84,89	0
1	SEP	D	15	10/11	0.93	0.14	64,73,79,85	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. 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(\AA^2)	Q<0.9
3	GOL	E	505	6/6	0.83	0.17	51,68,74,76	0
3	GOL	A	506	6/6	0.85	0.17	41,60,71,72	0
3	GOL	D	505	6/6	0.86	0.14	41,45,47,52	0
2	PO4	D	501	5/5	0.87	0.15	55,57,79,85	5
2	PO4	D	503	5/5	0.87	0.22	51,51,57,63	5
2	PO4	D	504	5/5	0.87	0.24	61,62,66,84	5
2	PO4	C	504	5/5	0.88	0.13	52,54,67,84	5
2	PO4	A	504	5/5	0.90	0.11	41,58,62,73	5
2	PO4	E	503	5/5	0.90	0.13	44,52,67,73	5
3	GOL	B	502	6/6	0.90	0.20	42,49,59,60	0
2	PO4	E	502	5/5	0.91	0.20	44,51,64,67	5
3	GOL	C	505	6/6	0.91	0.15	33,43,55,73	0
2	PO4	A	501	5/5	0.92	0.20	46,53,65,71	5
2	PO4	C	501	5/5	0.93	0.19	59,59,73,80	5
3	GOL	A	505	6/6	0.93	0.17	29,35,40,40	0
2	PO4	F	501	5/5	0.94	0.12	43,61,69,78	0
3	GOL	C	506	6/6	0.94	0.22	45,65,72,79	0
3	GOL	E	504	6/6	0.94	0.18	38,49,68,74	0
2	PO4	C	502	5/5	0.94	0.15	47,52,71,78	5
2	PO4	C	503	5/5	0.95	0.12	40,46,58,65	0
2	PO4	E	501	5/5	0.96	0.10	42,43,67,75	0
2	PO4	D	502	5/5	0.97	0.12	47,58,64,65	0
2	PO4	A	503	5/5	0.97	0.08	41,55,60,64	0
2	PO4	B	501	5/5	0.98	0.08	45,48,55,57	0
2	PO4	A	502	5/5	0.98	0.11	36,39,44,46	0

6.5 Other polymers

There are no such residues in this entry.