



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2017 – 03:34 AM EST

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 : unknown
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

<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 : rb-20030345
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) : rb-20030345

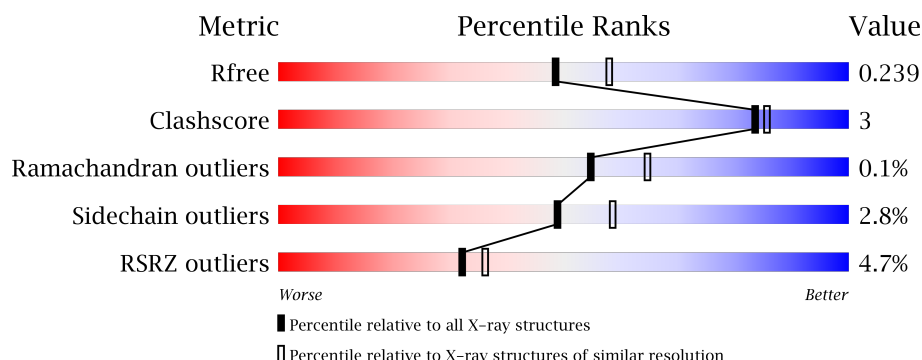
1 Overall quality at a glance

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}	100719	1062 (2.26-2.26)
Clashscore	112137	1178 (2.26-2.26)
Ramachandran outliers	110173	1145 (2.26-2.26)
Sidechain outliers	110143	1146 (2.26-2.26)
RSRZ outliers	101464	1066 (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. 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>0.1%</div> <div> <div></div> <div>89%</div> <div>7%</div> <div>..</div> </div> </div>
1	B	485	<div> <div>3%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>..</div> </div> </div>
1	C	485	<div> <div>2%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>..</div> </div> </div>
1	D	485	<div> <div>3%</div> <div> <div></div> <div>90%</div> <div>7%</div> <div>.</div> </div> </div>
1	E	485	<div> <div>5%</div> <div> <div></div> <div>91%</div> <div>6%</div> <div>.</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	485	

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	A	506	-	-	-	X
3	GOL	C	506	-	-	-	X

2 Entry composition [i](#)

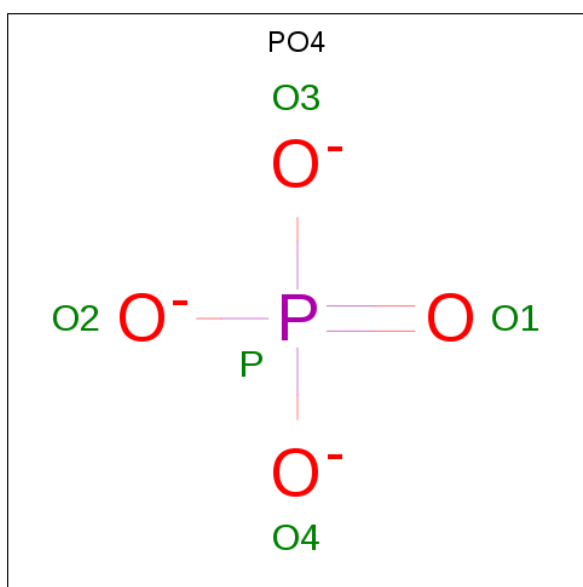
There are 4 unique types of molecules in this entry. The entry contains 22473 atoms, of which 0 are hydrogens and 0 are deuteriums.

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		

Continued on next page...

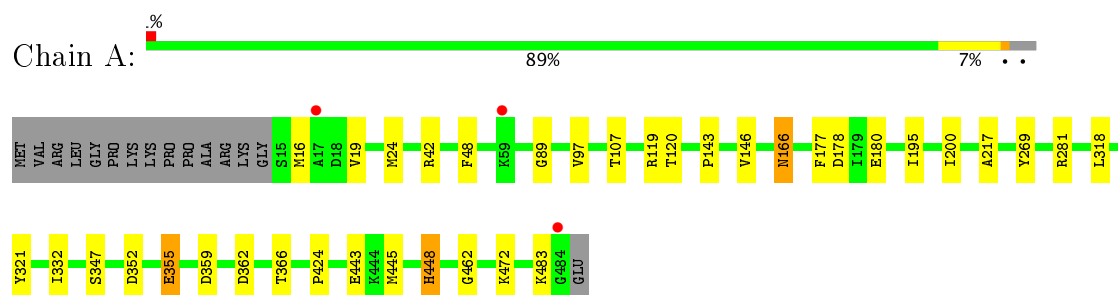
Continued from previous page...

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

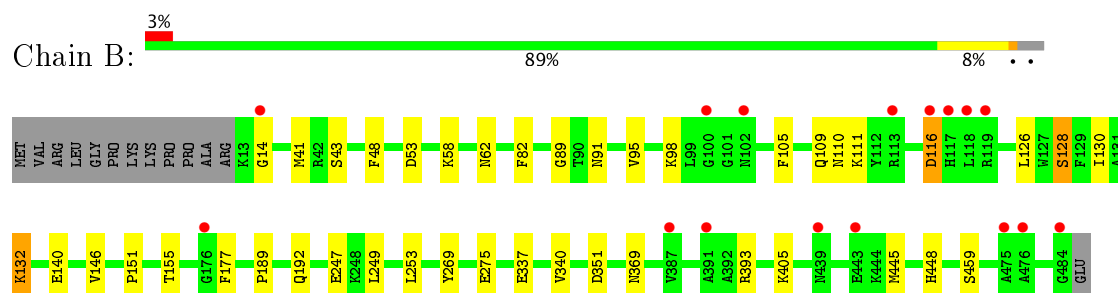
3 Residue-property plots [i](#)

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.

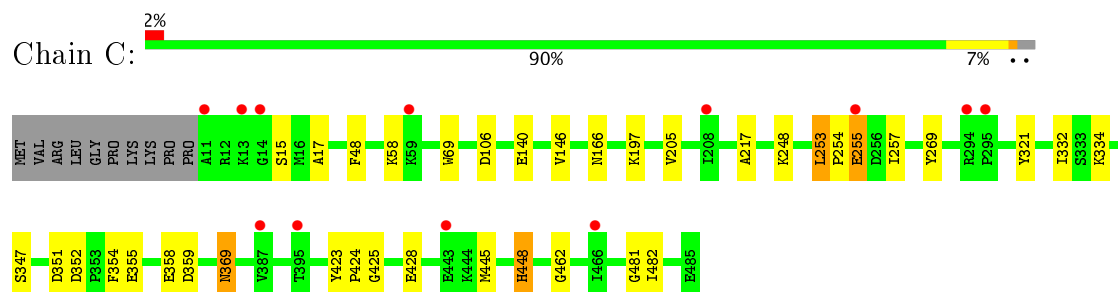
• Molecule 1: Hexokinase



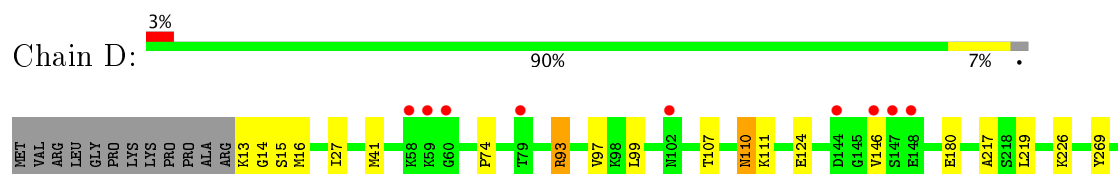
• Molecule 1: Hexokinase

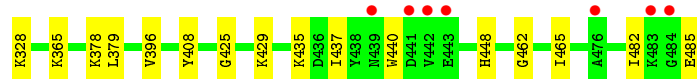


• Molecule 1: Hexokinase

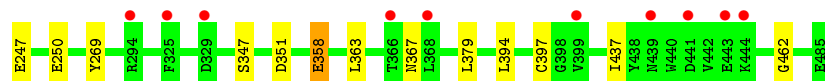
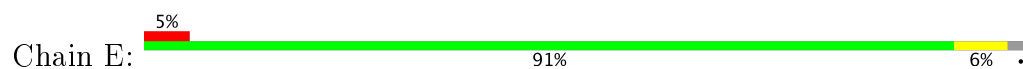


• Molecule 1: Hexokinase

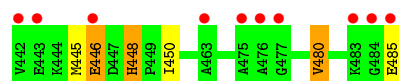
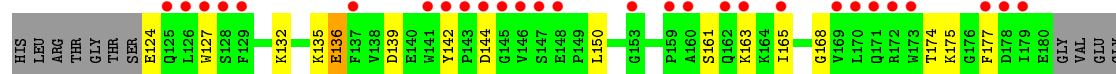
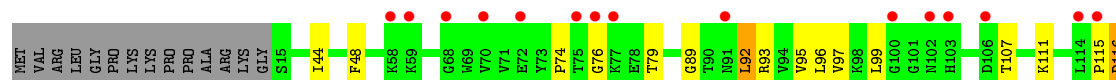
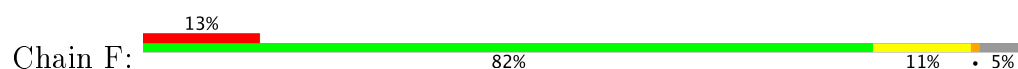




- Molecule 1: Hexokinase



- 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 (1.01%)	DCC
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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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%)	51	60
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%)	51	60
All	All	2805/2910 (96%)	2679 (96%)	124 (4%)	2 (0%)	55	65

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%)	49	58
1	B	402/411 (98%)	391 (97%)	11 (3%)	50	60
1	C	402/411 (98%)	391 (97%)	11 (3%)	50	60
1	D	401/411 (98%)	392 (98%)	9 (2%)	57	67
1	E	400/411 (97%)	389 (97%)	11 (3%)	49	58
1	F	392/411 (95%)	378 (96%)	14 (4%)	40	49
All	All	2397/2466 (97%)	2330 (97%)	67 (3%)	49	58

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	A	15	1	9,9,10	0.50	0	9,12,14	1.67	2 (22%)
1	SEP	B	15	1	9,9,10	0.76	0	9,12,14	3.51	4 (44%)
1	SEP	C	15	1	9,9,10	0.63	0	9,12,14	1.24	0
1	SEP	D	15	1	9,9,10	0.80	0	9,12,14	2.19	1 (11%)
1	SEP	E	15	1	9,9,10	0.63	0	9,12,14	1.43	1 (11%)
1	SEP	F	15	1	9,9,10	0.58	0	9,12,14	1.91	3 (33%)

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	A	15	1	-	0/5/8/10	0/0/0/0
1	SEP	B	15	1	-	0/5/8/10	0/0/0/0
1	SEP	C	15	1	-	0/5/8/10	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	SEP	D	15	1	-	0/5/8/10	0/0/0/0
1	SEP	E	15	1	-	0/5/8/10	0/0/0/0
1	SEP	F	15	1	-	0/5/8/10	0/0/0/0

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	O2P-P-OG	-4.19	95.57	106.73
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	B	15	SEP	O3P-P-O2P	2.01	115.74	107.61
1	F	15	SEP	O3P-P-O2P	2.14	116.26	107.61
1	B	15	SEP	OG-P-O1P	2.57	113.69	106.47
1	E	15	SEP	OG-CB-CA	2.63	110.76	108.17
1	A	15	SEP	OG-CB-CA	2.85	110.98	108.17
1	F	15	SEP	OG-CB-CA	3.81	111.92	108.17
1	D	15	SEP	OG-CB-CA	5.94	114.02	108.17
1	B	15	SEP	OG-CB-CA	8.82	116.87	108.17

There are no chirality outliers.

There are no torsion outliers.

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	A	501	-	4,4,4	0.68	0	6,6,6	0.46	0
2	PO4	A	502	-	4,4,4	0.97	0	6,6,6	1.11	1 (16%)
2	PO4	A	503	-	4,4,4	0.85	0	6,6,6	0.75	0
2	PO4	A	504	-	4,4,4	0.72	0	6,6,6	0.45	0
3	GOL	A	505	-	5,5,5	0.41	0	5,5,5	1.07	0
3	GOL	A	506	-	5,5,5	0.51	0	5,5,5	0.51	0
2	PO4	B	501	-	4,4,4	0.78	0	6,6,6	1.20	1 (16%)
3	GOL	B	502	-	5,5,5	0.25	0	5,5,5	1.06	0
2	PO4	C	501	-	4,4,4	0.71	0	6,6,6	0.47	0
2	PO4	C	502	-	4,4,4	0.69	0	6,6,6	0.38	0
2	PO4	C	503	-	4,4,4	0.62	0	6,6,6	0.68	0
2	PO4	C	504	-	4,4,4	0.59	0	6,6,6	0.58	0
3	GOL	C	505	-	5,5,5	0.43	0	5,5,5	0.79	0
3	GOL	C	506	-	5,5,5	0.42	0	5,5,5	0.40	0
2	PO4	D	501	-	4,4,4	0.75	0	6,6,6	0.44	0
2	PO4	D	502	-	4,4,4	0.78	0	6,6,6	0.61	0
2	PO4	D	503	-	4,4,4	0.73	0	6,6,6	0.47	0
2	PO4	D	504	-	4,4,4	0.70	0	6,6,6	0.47	0
3	GOL	D	505	-	5,5,5	0.48	0	5,5,5	0.38	0
2	PO4	E	501	-	4,4,4	0.79	0	6,6,6	0.73	0
2	PO4	E	502	-	4,4,4	0.68	0	6,6,6	0.92	0
2	PO4	E	503	-	4,4,4	0.79	0	6,6,6	0.43	0
3	GOL	E	504	-	5,5,5	0.34	0	5,5,5	0.52	0
3	GOL	E	505	-	5,5,5	0.36	0	5,5,5	0.46	0
2	PO4	F	501	-	4,4,4	0.75	0	6,6,6	0.63	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	PO4	A	501	-	-	0/0/0/0	0/0/0/0
2	PO4	A	502	-	-	0/0/0/0	0/0/0/0
2	PO4	A	503	-	-	0/0/0/0	0/0/0/0
2	PO4	A	504	-	-	0/0/0/0	0/0/0/0
3	GOL	A	505	-	-	0/4/4/4	0/0/0/0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	506	-	-	0/4/4/4	0/0/0/0
2	PO4	B	501	-	-	0/0/0/0	0/0/0/0
3	GOL	B	502	-	-	0/4/4/4	0/0/0/0
2	PO4	C	501	-	-	0/0/0/0	0/0/0/0
2	PO4	C	502	-	-	0/0/0/0	0/0/0/0
2	PO4	C	503	-	-	0/0/0/0	0/0/0/0
2	PO4	C	504	-	-	0/0/0/0	0/0/0/0
3	GOL	C	505	-	-	0/4/4/4	0/0/0/0
3	GOL	C	506	-	-	0/4/4/4	0/0/0/0
2	PO4	D	501	-	-	0/0/0/0	0/0/0/0
2	PO4	D	502	-	-	0/0/0/0	0/0/0/0
2	PO4	D	503	-	-	0/0/0/0	0/0/0/0
2	PO4	D	504	-	-	0/0/0/0	0/0/0/0
3	GOL	D	505	-	-	0/4/4/4	0/0/0/0
2	PO4	E	501	-	-	0/0/0/0	0/0/0/0
2	PO4	E	502	-	-	0/0/0/0	0/0/0/0
2	PO4	E	503	-	-	0/0/0/0	0/0/0/0
3	GOL	E	504	-	-	0/4/4/4	0/0/0/0
3	GOL	E	505	-	-	0/4/4/4	0/0/0/0
2	PO4	F	501	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	502	PO4	O3-P-O2	2.05	115.43	107.90
2	B	501	PO4	O4-P-O2	2.13	115.71	107.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	505	GOL	1	0
2	E	501	PO4	1	0
3	E	504	GOL	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	469/485 (96%)	-0.37	3 (0%) 89 89	23, 34, 56, 81	0
1	B	471/485 (97%)	-0.11	16 (3%) 46 49	27, 41, 74, 102	0
1	C	474/485 (97%)	-0.05	12 (2%) 58 61	19, 42, 80, 98	0
1	D	472/485 (97%)	-0.13	16 (3%) 46 49	25, 46, 74, 105	0
1	E	470/485 (96%)	0.08	22 (4%) 32 36	23, 52, 97, 156	0
1	F	459/485 (94%)	0.57	64 (13%) 3 3	25, 59, 115, 146	0
All	All	2815/2910 (96%)	-0.00	133 (4%) 32 36	19, 44, 92, 156	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	143	PRO	8.4
1	F	144	ASP	7.8
1	F	165	ILE	7.4
1	F	179	ILE	7.2
1	E	329	ASP	6.8
1	F	146	VAL	5.9
1	F	477	GLY	5.9
1	F	147	SER	5.7
1	F	475	ALA	5.7
1	F	177	PHE	5.6
1	F	476	ALA	5.3
1	F	170	LEU	5.1
1	F	173	TRP	4.9
1	F	159	PRO	4.9
1	F	126	LEU	4.7
1	F	128	SER	4.7
1	F	484	GLY	4.6
1	D	443	GLU	4.5
1	F	251	GLY	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	172	ARG	4.5
1	F	145	GLY	4.3
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	F	59	LYS	3.9
1	D	148	GLU	3.8
1	E	16	MET	3.8
1	C	11	ALA	3.7
1	E	17	ALA	3.7
1	D	59	LYS	3.7
1	D	147	SER	3.4
1	F	260	ASP	3.4
1	D	144	ASP	3.4
1	E	59	LYS	3.3
1	F	178	ASP	3.2
1	F	163	LYS	3.2
1	F	76	GLY	3.2
1	D	58	LYS	3.2
1	E	443	GLU	3.1
1	E	21	ALA	3.1
1	F	58	LYS	3.1
1	F	187	VAL	3.1
1	F	75	THR	3.1
1	F	446	GLU	3.1
1	F	442	VAL	3.0
1	F	171	GLN	3.0
1	F	441	ASP	3.0
1	B	14	GLY	3.0
1	B	176	GLY	3.0
1	F	169	VAL	2.9
1	C	294	ARG	2.9
1	A	484	GLY	2.8
1	F	77	LYS	2.8
1	B	100	GLY	2.8
1	F	153	GLY	2.8
1	E	439	ASN	2.8
1	E	60	GLY	2.7
1	B	117	HIS	2.7
1	D	476	ALA	2.7
1	E	22	ASN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	325	PHE	2.6
1	B	387	VAL	2.6
1	F	103	HIS	2.6
1	F	483	LYS	2.6
1	A	17	ALA	2.6
1	F	247	GLU	2.6
1	E	444	LYS	2.6
1	E	25	GLU	2.5
1	C	387	VAL	2.5
1	E	441	ASP	2.5
1	F	409	LYS	2.5
1	F	148	GLU	2.5
1	F	443	GLU	2.5
1	E	20	PRO	2.5
1	F	106	ASP	2.5
1	F	137	PHE	2.5
1	D	79	THR	2.5
1	D	483	LYS	2.5
1	C	295	PRO	2.4
1	F	102	ASN	2.4
1	B	476	ALA	2.4
1	D	442	VAL	2.4
1	B	439	ASN	2.4
1	F	259	PRO	2.4
1	C	466	ILE	2.4
1	B	443	GLU	2.4
1	D	146	VAL	2.4
1	E	208	ILE	2.3
1	F	70	VAL	2.3
1	B	113	ARG	2.3
1	E	19	VAL	2.3
1	F	72	GLU	2.3
1	B	391	ALA	2.3
1	D	441	ASP	2.3
1	F	127	TRP	2.3
1	B	119	ARG	2.3
1	E	18	ASP	2.3
1	B	116	ASP	2.3
1	F	125	GLN	2.3
1	F	162	GLN	2.3
1	B	118	LEU	2.2
1	C	59	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	294	ARG	2.2
1	F	238	ALA	2.2
1	F	100	GLY	2.2
1	F	91	ASN	2.2
1	C	255	GLU	2.2
1	F	115	PRO	2.2
1	F	129	PHE	2.2
1	B	484	GLY	2.2
1	F	485	GLU	2.2
1	C	13	LYS	2.2
1	E	58	LYS	2.2
1	C	14	GLY	2.2
1	D	60	GLY	2.2
1	D	484	GLY	2.2
1	C	443	GLU	2.2
1	B	102	ASN	2.2
1	F	196	GLU	2.2
1	E	399	VAL	2.1
1	F	160	ALA	2.1
1	E	366	THR	2.1
1	C	208	ILE	2.1
1	D	439	ASN	2.1
1	B	475	ALA	2.1
1	A	59	LYS	2.1
1	C	395	THR	2.1
1	F	463	ALA	2.1
1	D	102	ASN	2.0
1	F	68	GLY	2.0
1	F	189	PRO	2.0
1	E	368	LEU	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. 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
1	SEP	C	15	10/11	0.82	0.28	-	83,95,111,115	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	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
1	SEP	E	15	10/11	0.84	0.30	-	103,126,142,144	0
1	SEP	B	15	10/11	0.84	0.15	-	68,81,87,91	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	GOL	C	506	6/6	0.94	0.22	5.30	45,65,72,79	0
3	GOL	A	506	6/6	0.85	0.17	3.32	41,60,71,72	0
3	GOL	B	502	6/6	0.90	0.20	0.93	42,49,59,60	0
3	GOL	A	505	6/6	0.93	0.17	0.90	29,35,40,40	0
3	GOL	D	505	6/6	0.86	0.14	0.88	41,45,47,52	0
3	GOL	E	504	6/6	0.94	0.18	0.85	38,49,68,74	0
2	PO4	A	502	5/5	0.98	0.11	-0.08	36,39,44,46	0
3	GOL	C	505	6/6	0.91	0.15	-0.26	33,43,55,73	0
2	PO4	B	501	5/5	0.98	0.08	-	45,48,55,57	0
2	PO4	E	502	5/5	0.91	0.20	-	44,51,64,67	5
2	PO4	C	502	5/5	0.94	0.15	-	47,52,71,78	5
2	PO4	F	501	5/5	0.94	0.12	-	43,61,69,78	0
2	PO4	C	501	5/5	0.93	0.19	-	59,59,73,80	5
2	PO4	D	502	5/5	0.97	0.12	-	47,58,64,65	0
2	PO4	A	504	5/5	0.89	0.12	-	41,58,62,73	5
2	PO4	A	501	5/5	0.92	0.20	-	46,53,65,71	5
2	PO4	D	501	5/5	0.87	0.15	-	55,57,79,85	5
2	PO4	C	503	5/5	0.96	0.12	-	40,46,58,65	0
2	PO4	C	504	5/5	0.87	0.13	-	52,54,67,84	5
2	PO4	D	503	5/5	0.88	0.22	-	51,51,57,63	5
2	PO4	A	503	5/5	0.97	0.08	-	41,55,60,64	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	PO4	E	503	5/5	0.90	0.13	-	44,52,67,73	5
2	PO4	D	504	5/5	0.87	0.24	-	61,62,66,84	5
2	PO4	E	501	5/5	0.96	0.10	-	42,43,67,75	0
3	GOL	E	505	6/6	0.83	0.17	-	51,68,74,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.