Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 11:40 AM EDT

PDB ID	:	6N8G
Title	:	IRAK4 bound to benzoxazole compound
Authors	:	Larsen, N.A.; Bloudoff, K.; Subramanian, V.; Dobrzanska, M.; Gluza, K.
Deposited on	:	2018-11-29
Resolution	:	2.00 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

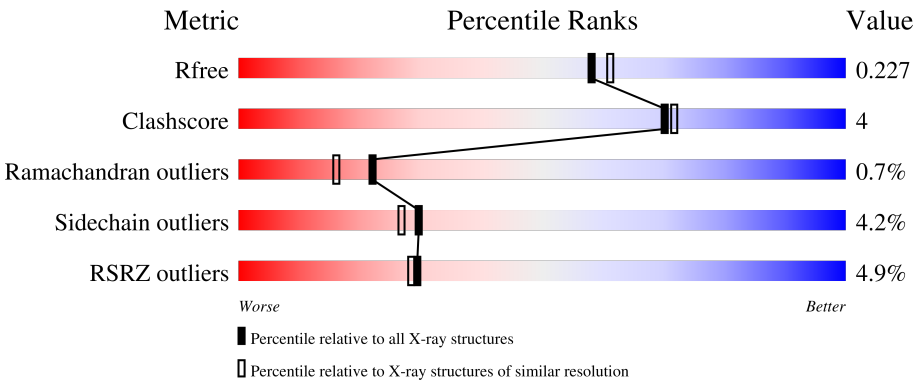
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	297	4% 82% 12% • •
1	B	297	6% 85% 11% • •
1	C	297	3% 83% 13% • •
1	D	297	5% 80% 12% • 6%

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
1	TPO	A	342	-	-	-	X

2 Entry composition (i)

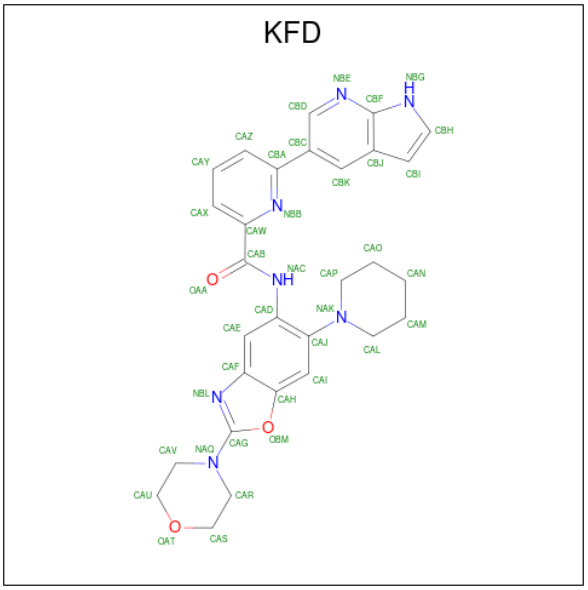
There are 3 unique types of molecules in this entry. The entry contains 9674 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	288	2268	1420	381	450	3	14	0	0	0
1	B	286	2253	1409	379	447	3	15	0	1	0
1	C	289	2302	1444	386	455	3	14	0	3	0
1	D	280	2199	1375	372	435	3	14	0	0	0

- Molecule 2 is N-[2-(morpholin-4-yl)-6-(piperidin-1-yl)-1,3-benzoxazol-5-yl]-6-(1H-pyrrolo[2,3-b]pyridin-5-yl)pyridine-2-carboxamide (three-letter code: KFD) (formula: $C_{29}H_{29}N_7O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	39	29	7	3	0	0
2	B	1	39	29	7	3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	C	1	39	29	7	3	0	0
			Total	C	N	O		
2	D	1	39	29	7	3	0	0

- Molecule 3 is water.

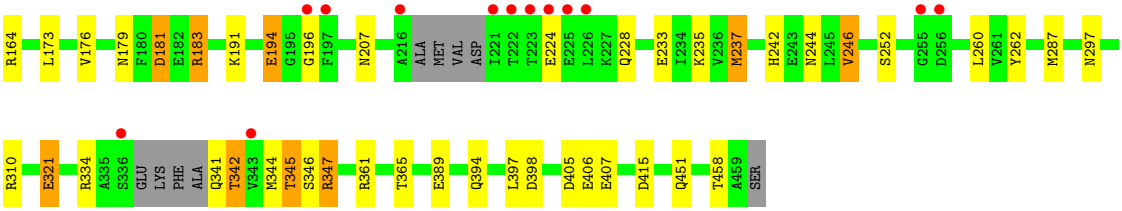
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	144	144	144	0	0
			Total	O		
3	B	95	95	95	0	0
			Total	O		
3	C	161	161	161	0	0
			Total	O		
3	D	96	96	96	0	0

3 Residue-property plots (i)

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.

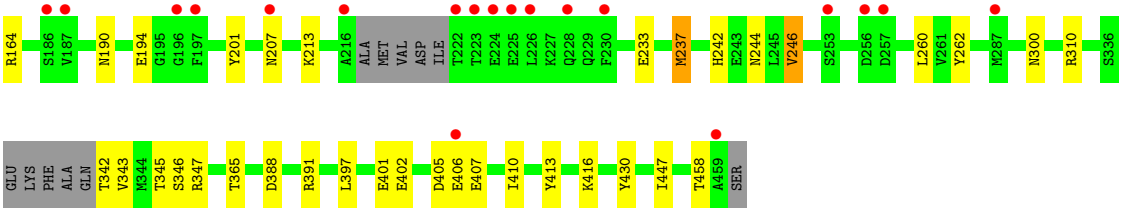
• Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain A:



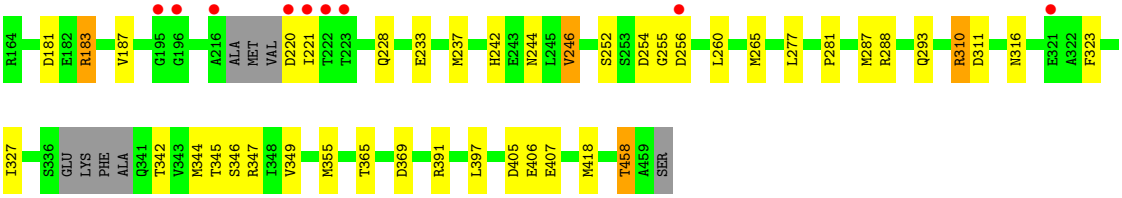
• Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain B:



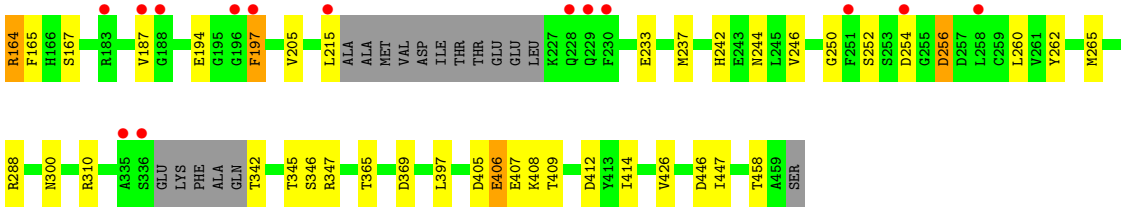
• Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain C:



• Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain D:


R164
F165
H166
S167
R183
V187
G188
E194
G195
G196
F197
V205
L215
ALA
ALA
MET
VAL
ASP
ILE
THR
THR
GLU
GLU
LEU
K227
Q228
Q229
F230
E233
M237
H242
E243
N244
L245
V246
G250
F251
S252
S253
D254
G255
D256
D257
L258
C259
L260
V261
Y262
M265
R288
N300
R310
A335
S336
GLU
LYS
PHE
ALA
GLN
T342
T345
S346
R347
T365
D369
L397
D405
E406
E407
K408
T409
D412
Y413
I414
V426
D446
I447
T458
A459
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	142.96Å 141.93Å 88.09Å 90.00° 124.58° 90.00°	Depositor
Resolution (Å)	90.60 – 2.00 49.30 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (90.60-2.00) 99.8 (49.30-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.174 , 0.220 0.184 , 0.227	Depositor DCC
R_{free} test set	4894 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	40.2	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 48.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	9674	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.28% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

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

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	2/2271 (0.1%)	1.10	11/3059 (0.4%)
1	B	0.92	0/2259	0.98	4/3043 (0.1%)
1	C	1.03	2/2316 (0.1%)	1.13	14/3119 (0.4%)
1	D	0.91	0/2202	0.99	5/2967 (0.2%)
All	All	0.97	4/9048 (0.0%)	1.05	34/12188 (0.3%)

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	B	0	1
1	C	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	316	ASN	CA-CB	7.21	1.71	1.53
1	A	252	SER	CB-OG	-6.27	1.34	1.42
1	A	183	ARG	CD-NE	-6.08	1.36	1.46
1	C	183	ARG	CD-NE	-5.32	1.37	1.46

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	183	ARG	NE-CZ-NH1	17.86	129.23	120.30
1	A	183	ARG	NE-CZ-NH2	-16.43	112.09	120.30
1	A	183	ARG	NE-CZ-NH1	15.96	128.28	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	183	ARG	NE-CZ-NH2	-13.86	113.37	120.30
1	D	265	MET	CG-SD-CE	10.11	116.38	100.20
1	C	237	MET	CG-SD-CE	-9.68	84.72	100.20
1	B	310	ARG	NE-CZ-NH1	8.27	124.44	120.30
1	C	246	VAL	CG1-CB-CG2	8.02	123.74	110.90
1	B	310	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	C	369	ASP	CB-CG-OD1	7.46	125.02	118.30
1	D	369	ASP	CB-CG-OD1	7.46	125.01	118.30
1	D	310	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	C	183	ARG	CD-NE-CZ	6.39	132.55	123.60
1	B	237	MET	CG-SD-CE	-6.37	90.00	100.20
1	C	369	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	B	246	VAL	CG1-CB-CG2	6.14	120.73	110.90
1	A	237	MET	CG-SD-CE	-5.95	90.67	100.20
1	C	311	ASP	CB-CG-OD1	5.86	123.57	118.30
1	A	415	ASP	CB-CG-OD1	5.84	123.56	118.30
1	D	288	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	C	265	MET	CG-SD-CE	5.77	109.43	100.20
1	C	355	MET	CG-SD-CE	-5.72	91.04	100.20
1	C	316	ASN	CB-CG-OD1	-5.72	110.16	121.60
1	C	310	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	347	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	A	310	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	361	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	246	VAL	CG1-CB-CG2	5.57	119.82	110.90
1	C	246	VAL	CA-CB-CG1	5.53	119.20	110.90
1	D	446	ASP	CB-CG-OD1	5.44	123.19	118.30
1	A	181	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	C	288	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	246	VAL	CB-CA-C	5.02	120.95	111.40
1	A	181	ASP	CB-CG-OD1	5.02	122.81	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	207	ASN	Peptide
1	C	255	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2268	0	2220	22	0
1	B	2253	0	2211	14	0
1	C	2302	0	2258	14	0
1	D	2199	0	2150	17	0
2	A	39	0	0	0	0
2	B	39	0	0	1	0
2	C	39	0	0	0	0
2	D	39	0	0	0	0
3	A	144	0	0	4	0
3	B	95	0	0	1	0
3	C	161	0	0	2	0
3	D	96	0	0	3	0
All	All	9674	0	8839	65	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 4.

All (65) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ASN:HB3	3:A:696:HOH:O	1.77	0.84
1:C:242:HIS:HD2	1:C:244:ASN:H	1.24	0.82
1:D:405:ASP:O	1:D:407:GLU:N	2.17	0.77
1:C:181:ASP:OD1	1:C:183:ARG:HD3	1.90	0.72
1:C:233:GLU:HG2	1:C:260:LEU:HD13	1.73	0.71
1:C:242:HIS:CD2	1:C:244:ASN:H	2.09	0.69
1:A:242:HIS:CD2	1:A:244:ASN:H	2.10	0.69
1:D:242:HIS:CD2	1:D:244:ASN:H	2.13	0.67
1:B:242:HIS:CD2	1:B:244:ASN:H	2.13	0.66
1:A:242:HIS:HD2	1:A:244:ASN:H	1.43	0.65
1:A:181:ASP:OD1	1:A:183:ARG:HD3	1.99	0.62
1:A:321:GLU:HG2	1:C:281:PRO:HD3	1.82	0.62
1:D:242:HIS:HD2	1:D:244:ASN:H	1.48	0.61
1:A:181:ASP:OD1	1:A:183:ARG:CD	2.49	0.60
1:A:397:LEU:C	1:A:397:LEU:HD12	2.23	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:409:THR:HG22	1:D:412:ASP:OD2	2.04	0.58
1:C:405:ASP:O	1:C:407:GLU:N	2.37	0.58
1:C:327:ILE:HG23	3:C:658:HOH:O	2.06	0.56
1:D:407:GLU:O	1:D:408:LYS:HG2	2.07	0.55
1:D:215:LEU:C	3:D:653:HOH:O	2.45	0.54
1:D:397:LEU:C	1:D:397:LEU:HD12	2.28	0.54
1:D:197:PHE:HA	3:D:637:HOH:O	2.07	0.54
1:C:391:ARG:HD3	3:C:686:HOH:O	2.08	0.53
1:D:237:MET:HE3	1:D:262:TYR:HE2	1.73	0.53
1:B:237:MET:CE	1:B:262:TYR:HE2	2.22	0.53
1:A:233:GLU:HG2	1:A:260:LEU:HD13	1.90	0.52
1:C:397:LEU:HD12	1:C:397:LEU:C	2.30	0.52
1:B:405:ASP:O	1:B:407:GLU:N	2.43	0.51
1:D:300:ASN:HA	1:D:447:ILE:HG21	1.94	0.50
1:A:207:ASN:O	3:A:601:HOH:O	2.19	0.50
1:A:233:GLU:OE2	3:A:602:HOH:O	2.19	0.50
1:A:228:GLN:CB	3:A:736:HOH:O	2.59	0.49
1:A:297:ASN:ND2	1:A:451:GLN:OE1	2.45	0.49
1:D:164:ARG:HD2	3:D:673:HOH:O	2.13	0.48
1:A:191:LYS:NZ	1:A:194:GLU:OE2	2.34	0.48
1:A:237:MET:CE	1:A:262:TYR:HE2	2.27	0.47
1:B:410:ILE:HD13	1:B:430:TYR:CD1	2.49	0.47
1:D:165:PHE:HB3	1:D:250:GLY:HA2	1.97	0.46
1:D:256:ASP:N	1:D:256:ASP:OD1	2.48	0.46
1:B:242:HIS:HD2	1:B:244:ASN:H	1.62	0.46
1:C:233:GLU:HG2	1:C:260:LEU:CD1	2.45	0.46
1:A:181:ASP:OD1	1:A:183:ARG:HD2	2.17	0.45
1:B:416:LYS:HB3	1:C:277:LEU:HD12	1.99	0.45
1:B:233:GLU:HG2	1:B:260:LEU:HD13	1.97	0.45
1:A:405:ASP:O	1:A:407:GLU:N	2.50	0.45
1:D:233:GLU:HG2	1:D:260:LEU:HD13	1.98	0.45
1:D:405:ASP:C	1:D:407:GLU:H	2.21	0.44
1:B:190:ASN:O	1:B:201:TYR:HA	2.18	0.44
1:B:300:ASN:HA	1:B:447:ILE:HG21	2.00	0.43
1:B:213:LYS:NZ	2:B:501:KFD:NBE	2.66	0.43
1:B:397:LEU:C	1:B:397:LEU:HD12	2.39	0.43
1:A:287:MET:HA	1:A:287:MET:HE2	2.00	0.43
1:A:334:ARG:NH2	1:A:345:TPO:O3P	2.36	0.43
1:A:397:LEU:HD12	1:A:398:ASP:N	2.34	0.42
1:A:341:GLN:O	1:A:342:TPO:C	2.68	0.42
1:D:414:ILE:CD1	1:D:426:VAL:HG11	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:LEU:HA	1:A:176:VAL:HG22	2.02	0.41
1:C:310:ARG:NH1	1:C:349:VAL:HG22	2.35	0.41
1:B:402:GLU:OE1	1:B:413:TYR:OH	2.34	0.41
1:C:293:GLN:HE22	1:C:458:THR:HG21	1.86	0.41
1:B:401:GLU:HG3	3:B:605:HOH:O	2.19	0.41
1:A:389:GLU:HA	1:A:394:GLN:HE21	1.86	0.41
1:B:388:ASP:HB3	1:B:391:ARG:HB3	2.03	0.41
1:D:237:MET:CE	1:D:262:TYR:HE2	2.33	0.40
1:C:287:MET:CE	1:C:323:PHE:HB2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	279/297 (94%)	266 (95%)	11 (4%)	2 (1%)	22 16
1	B	279/297 (94%)	271 (97%)	7 (2%)	1 (0%)	34 30
1	C	283/297 (95%)	270 (95%)	11 (4%)	2 (1%)	22 16
1	D	272/297 (92%)	261 (96%)	8 (3%)	3 (1%)	14 8
All	All	1113/1188 (94%)	1068 (96%)	37 (3%)	8 (1%)	22 16

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	254	ASP
1	C	406	GLU
1	D	197	PHE
1	D	406	GLU
1	A	406	GLU
1	B	406	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	196	GLY
1	D	187	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	246/255 (96%)	236 (96%)	10 (4%)	30	28
1	B	245/255 (96%)	238 (97%)	7 (3%)	42	43
1	C	251/255 (98%)	239 (95%)	12 (5%)	25	22
1	D	238/255 (93%)	226 (95%)	12 (5%)	24	20
All	All	980/1020 (96%)	939 (96%)	41 (4%)	30	27

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	ARG
1	A	194	GLU
1	A	224	GLU
1	A	235	LYS
1	A	246	VAL
1	A	321	GLU
1	A	344	MET
1	A	347	ARG
1	A	365	THR
1	A	458	THR
1	B	164	ARG
1	B	194	GLU
1	B	246	VAL
1	B	343	VAL
1	B	347	ARG
1	B	365	THR
1	B	458	THR
1	C	187	VAL
1	C	220	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	221	ILE
1	C	228	GLN
1	C	246	VAL
1	C	252	SER
1	C	256	ASP
1	C	344	MET
1	C	347	ARG
1	C	365	THR
1	C	418	MET
1	C	458	THR
1	D	164	ARG
1	D	167	SER
1	D	194	GLU
1	D	205	VAL
1	D	246	VAL
1	D	252	SER
1	D	254	ASP
1	D	256	ASP
1	D	347	ARG
1	D	365	THR
1	D	406	GLU
1	D	458	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	HIS
1	A	286	HIS
1	A	293	GLN
1	A	297	ASN
1	A	394	GLN
1	A	451	GLN
1	B	207	ASN
1	B	242	HIS
1	B	293	GLN
1	B	297	ASN
1	B	394	GLN
1	B	451	GLN
1	C	242	HIS
1	C	293	GLN
1	C	297	ASN
1	C	394	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	451	GLN
1	C	452	GLN
1	D	242	HIS
1	D	297	ASN
1	D	451	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

12 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	TPO	C	345	1	8,10,11	1.26	1 (12%)	10,14,16	1.01	1 (10%)
1	TPO	D	345	1	8,10,11	1.14	1 (12%)	10,14,16	1.30	1 (10%)
1	TPO	B	345	1	8,10,11	1.17	1 (12%)	10,14,16	1.49	1 (10%)
1	SEP	B	346	1	8,9,10	0.71	0	8,12,14	1.56	1 (12%)
1	TPO	D	342	1	8,10,11	1.00	0	10,14,16	1.23	1 (10%)
1	SEP	A	346	1	8,9,10	0.67	0	8,12,14	1.54	1 (12%)
1	SEP	D	346	1	8,9,10	0.79	0	8,12,14	1.67	2 (25%)
1	TPO	B	342	1	8,10,11	1.19	1 (12%)	10,14,16	1.11	2 (20%)
1	TPO	A	342	1	8,10,11	1.41	1 (12%)	10,14,16	1.16	0
1	SEP	C	346	1	8,9,10	0.61	0	8,12,14	1.49	2 (25%)
1	TPO	A	345	1	8,10,11	1.24	1 (12%)	10,14,16	1.31	2 (20%)
1	TPO	C	342	1	8,10,11	1.03	1 (12%)	10,14,16	0.96	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
1	TPO	C	345	1	-	4/9/11/13	-
1	TPO	D	345	1	-	4/9/11/13	-
1	TPO	B	345	1	-	2/9/11/13	-
1	SEP	B	346	1	-	1/5/8/10	-
1	TPO	D	342	1	-	1/9/11/13	-
1	SEP	A	346	1	-	1/5/8/10	-
1	SEP	D	346	1	-	4/5/8/10	-
1	TPO	B	342	1	-	3/9/11/13	-
1	TPO	A	342	1	-	1/9/11/13	-
1	SEP	C	346	1	-	1/5/8/10	-
1	TPO	A	345	1	-	3/9/11/13	-
1	TPO	C	342	1	-	4/9/11/13	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	342	TPO	P-OG1	2.91	1.64	1.59
1	B	342	TPO	P-OG1	2.49	1.64	1.59
1	C	345	TPO	P-OG1	2.38	1.63	1.59
1	D	345	TPO	P-OG1	2.36	1.63	1.59
1	A	345	TPO	P-OG1	2.25	1.63	1.59
1	C	342	TPO	P-OG1	2.13	1.63	1.59
1	B	345	TPO	P-OG1	2.10	1.63	1.59

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	345	TPO	P-OG1-CB	-3.50	112.65	123.21
1	D	342	TPO	P-OG1-CB	-3.17	113.64	123.21
1	C	346	SEP	OG-CB-CA	3.08	111.15	108.14
1	D	346	SEP	P-OG-CB	3.03	126.64	118.30
1	A	346	SEP	OG-CB-CA	3.01	111.07	108.14
1	B	346	SEP	O3P-P-OG	-2.78	99.33	106.73
1	A	345	TPO	P-OG1-CB	-2.70	115.07	123.21
1	D	346	SEP	OG-CB-CA	2.58	110.65	108.14
1	D	345	TPO	P-OG1-CB	-2.50	115.65	123.21
1	B	342	TPO	P-OG1-CB	-2.17	116.65	123.21
1	C	345	TPO	P-OG1-CB	-2.16	116.68	123.21
1	B	342	TPO	CG2-CB-CA	2.14	117.38	113.16

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	346	SEP	O3P-P-O2P	2.03	115.39	107.64
1	A	345	TPO	CG2-CB-CA	2.01	117.13	113.16

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	A	345	TPO	CB-OG1-P-O1P
1	A	346	SEP	N-CA-CB-OG
1	B	342	TPO	N-CA-CB-OG1
1	B	342	TPO	O-C-CA-CB
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	O-C-CA-CB
1	B	346	SEP	N-CA-CB-OG
1	C	342	TPO	C-CA-CB-CG2
1	C	342	TPO	CB-OG1-P-O1P
1	C	345	TPO	N-CA-CB-OG1
1	C	345	TPO	CB-OG1-P-O1P
1	C	346	SEP	N-CA-CB-OG
1	D	342	TPO	O-C-CA-CB
1	D	345	TPO	N-CA-CB-OG1
1	D	345	TPO	O-C-CA-CB
1	D	345	TPO	CB-OG1-P-O1P
1	D	346	SEP	N-CA-CB-OG
1	D	346	SEP	CB-OG-P-O1P
1	D	346	SEP	CB-OG-P-O2P
1	D	346	SEP	CB-OG-P-O3P
1	A	342	TPO	CB-OG1-P-O3P
1	B	342	TPO	C-CA-CB-CG2
1	C	342	TPO	CA-CB-OG1-P
1	C	345	TPO	CA-CB-OG1-P
1	D	345	TPO	CA-CB-OG1-P
1	A	345	TPO	O-C-CA-CB
1	C	342	TPO	O-C-CA-CB
1	C	345	TPO	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	342	TPO	1	0
1	A	345	TPO	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	KFD	B	501	-	41,45,45	2.28	19 (46%)	50,64,64	2.13	13 (26%)
2	KFD	D	501	-	41,45,45	2.45	15 (36%)	50,64,64	2.03	14 (28%)
2	KFD	C	501	-	41,45,45	2.25	15 (36%)	50,64,64	1.90	13 (26%)
2	KFD	A	501	-	41,45,45	2.23	12 (29%)	50,64,64	1.98	12 (24%)

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	KFD	B	501	-	-	3/16/36/36	0/7/7/7
2	KFD	D	501	-	-	3/16/36/36	0/7/7/7
2	KFD	C	501	-	-	3/16/36/36	0/7/7/7
2	KFD	A	501	-	-	3/16/36/36	0/7/7/7

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	KFD	CBD-NBE	6.66	1.42	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	KFD	CBD-NBE	6.23	1.41	1.31
2	D	501	KFD	CAE-CAF	-6.16	1.32	1.41
2	A	501	KFD	CBC-CBA	-5.81	1.39	1.48
2	B	501	KFD	CBC-CBA	-5.76	1.39	1.48
2	A	501	KFD	CAE-CAF	-5.46	1.33	1.41
2	D	501	KFD	CBC-CBA	-5.11	1.40	1.48
2	D	501	KFD	CBD-NBE	5.00	1.39	1.31
2	D	501	KFD	CAD-NAC	-4.72	1.32	1.41
2	C	501	KFD	CBF-NBE	-4.32	1.31	1.37
2	C	501	KFD	CBC-CBA	-4.14	1.42	1.48
2	D	501	KFD	CAR-NAQ	4.08	1.53	1.46
2	D	501	KFD	CBJ-CBF	-3.99	1.32	1.43
2	C	501	KFD	CAE-CAF	-3.98	1.35	1.41
2	B	501	KFD	CBK-CBJ	-3.95	1.33	1.42
2	B	501	KFD	CAI-CAJ	3.92	1.44	1.38
2	D	501	KFD	CBK-CBJ	-3.87	1.33	1.42
2	B	501	KFD	CAE-CAF	-3.82	1.35	1.41
2	B	501	KFD	CAW-CAB	-3.64	1.41	1.50
2	D	501	KFD	CAJ-NAK	-3.62	1.33	1.41
2	B	501	KFD	CBF-NBE	-3.54	1.32	1.37
2	C	501	KFD	CBJ-CBF	-3.50	1.33	1.43
2	D	501	KFD	CAW-CAB	-3.48	1.42	1.50
2	C	501	KFD	CAR-NAQ	3.47	1.52	1.46
2	A	501	KFD	CBK-CBJ	-3.45	1.34	1.42
2	A	501	KFD	CAV-NAQ	3.42	1.52	1.46
2	C	501	KFD	CBK-CBJ	-3.30	1.34	1.42
2	B	501	KFD	CBJ-CBF	-3.27	1.34	1.43
2	C	501	KFD	CAI-CAJ	3.27	1.43	1.38
2	C	501	KFD	CAD-NAC	-3.27	1.35	1.41
2	B	501	KFD	CAI-CAH	-3.21	1.31	1.37
2	C	501	KFD	CAN-CAM	3.07	1.63	1.51
2	B	501	KFD	CAJ-NAK	-3.01	1.34	1.41
2	D	501	KFD	CAV-NAQ	2.99	1.51	1.46
2	A	501	KFD	CAW-CAB	-2.92	1.43	1.50
2	B	501	KFD	OAT-CAS	2.88	1.54	1.42
2	C	501	KFD	CAP-NAK	2.80	1.51	1.46
2	A	501	KFD	CBJ-CBF	-2.80	1.35	1.43
2	C	501	KFD	CAJ-NAK	-2.72	1.35	1.41
2	D	501	KFD	CAD-CAJ	2.54	1.43	1.40
2	B	501	KFD	CAR-CAS	2.52	1.60	1.50
2	A	501	KFD	CAD-CAJ	2.42	1.43	1.40
2	B	501	KFD	CAG-NBL	2.40	1.38	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	501	KFD	CAF-CAH	-2.39	1.34	1.42
2	B	501	KFD	CAV-NAQ	2.37	1.50	1.46
2	B	501	KFD	CBD-NBE	2.35	1.35	1.31
2	D	501	KFD	CAI-CAH	-2.35	1.33	1.37
2	B	501	KFD	CAV-CAU	2.35	1.59	1.50
2	A	501	KFD	CAF-NBL	-2.29	1.31	1.38
2	B	501	KFD	CAF-CAH	-2.28	1.34	1.42
2	D	501	KFD	CBF-NBE	-2.27	1.34	1.37
2	C	501	KFD	CAW-CAB	-2.26	1.45	1.50
2	B	501	KFD	OAT-CAU	2.25	1.51	1.42
2	B	501	KFD	CAO-CAN	-2.20	1.42	1.51
2	A	501	KFD	CAR-CAS	2.17	1.58	1.50
2	A	501	KFD	CAL-NAK	2.15	1.50	1.46
2	C	501	KFD	CAV-CAU	2.14	1.58	1.50
2	B	501	KFD	CAE-CAD	-2.12	1.33	1.37
2	C	501	KFD	CAF-CAH	-2.10	1.35	1.42
2	A	501	KFD	CBF-NBE	-2.04	1.34	1.37
2	D	501	KFD	CAV-CAU	2.04	1.58	1.50

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	501	KFD	CBC-CBD-NBE	-6.38	119.65	125.55
2	C	501	KFD	CBC-CBD-NBE	-5.57	120.39	125.55
2	D	501	KFD	CAX-CAW-NBB	-5.31	116.69	122.92
2	D	501	KFD	CBC-CBD-NBE	-5.25	120.69	125.55
2	A	501	KFD	CBC-CBD-NBE	-5.23	120.71	125.55
2	D	501	KFD	CBC-CBA-NBB	4.90	122.99	116.02
2	B	501	KFD	CAS-CAR-NAQ	-4.88	101.02	110.02
2	B	501	KFD	CAE-CAD-CAJ	-4.76	114.39	119.82
2	A	501	KFD	CAU-OAT-CAS	4.76	125.77	109.89
2	C	501	KFD	CBD-NBE-CBF	4.68	121.39	116.69
2	C	501	KFD	CAX-CAW-NBB	-4.60	117.53	122.92
2	A	501	KFD	CBC-CBA-NBB	4.52	122.45	116.02
2	A	501	KFD	CAV-NAQ-CAR	4.34	121.10	111.52
2	B	501	KFD	CBD-NBE-CBF	4.21	120.92	116.69
2	B	501	KFD	CAU-OAT-CAS	3.83	122.69	109.89
2	C	501	KFD	CAV-NAQ-CAR	3.81	119.93	111.52
2	A	501	KFD	CAX-CAW-NBB	-3.73	118.55	122.92
2	D	501	KFD	CBA-NBB-CAW	3.67	124.36	118.11
2	D	501	KFD	CAV-NAQ-CAR	3.58	119.42	111.52
2	D	501	KFD	CAN-CAM-CAL	-3.33	104.74	111.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	KFD	OAT-CAS-CAR	-3.33	104.47	111.80
2	B	501	KFD	CBC-CBA-NBB	3.31	120.72	116.02
2	D	501	KFD	CAB-CAW-NBB	3.28	122.63	117.42
2	B	501	KFD	CAE-CAF-CAH	3.21	124.36	121.12
2	A	501	KFD	CAP-NAK-CAL	3.19	118.55	111.52
2	B	501	KFD	OAT-CAS-CAR	3.17	118.77	111.80
2	C	501	KFD	CAY-CAX-CAW	3.15	122.44	118.63
2	A	501	KFD	CAY-CAX-CAW	3.10	122.38	118.63
2	B	501	KFD	CAX-CAW-NBB	-2.98	119.43	122.92
2	B	501	KFD	CAP-NAK-CAL	2.92	117.97	111.52
2	D	501	KFD	OAA-CAB-NAC	2.83	130.17	123.71
2	D	501	KFD	CAW-CAB-NAC	-2.80	107.24	114.04
2	A	501	KFD	OAT-CAS-CAR	2.77	117.90	111.80
2	D	501	KFD	CAP-NAK-CAJ	2.71	122.70	116.27
2	B	501	KFD	CBA-NBB-CAW	2.67	122.66	118.11
2	C	501	KFD	CBA-NBB-CAW	2.63	122.59	118.11
2	B	501	KFD	CAJ-CAI-CAH	-2.54	117.04	119.46
2	D	501	KFD	CAS-CAR-NAQ	-2.54	105.34	110.02
2	D	501	KFD	CAZ-CBA-NBB	-2.52	118.70	121.97
2	A	501	KFD	CBA-NBB-CAW	2.51	122.39	118.11
2	C	501	KFD	CAJ-CAD-NAC	-2.42	114.05	118.58
2	C	501	KFD	CAS-CAR-NAQ	-2.32	105.74	110.02
2	D	501	KFD	CAU-OAT-CAS	2.32	117.62	109.89
2	B	501	KFD	CAE-CAD-NAC	2.22	128.66	121.78
2	A	501	KFD	CAB-CAW-NBB	2.19	120.91	117.42
2	D	501	KFD	CAY-CAX-CAW	2.15	121.22	118.63
2	A	501	KFD	CAN-CAM-CAL	-2.12	107.09	111.19
2	A	501	KFD	CAZ-CAY-CAX	-2.11	117.25	120.25
2	C	501	KFD	CAB-CAW-NBB	2.05	120.68	117.42
2	C	501	KFD	CAN-CAO-CAP	-2.04	107.23	111.19
2	C	501	KFD	OAT-CAU-CAV	-2.01	107.36	111.80
2	C	501	KFD	CAZ-CAY-CAX	-2.01	117.40	120.25

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	KFD	CAI-CAJ-NAK-CAP
2	A	501	KFD	CAI-CAJ-NAK-CAL
2	C	501	KFD	CAI-CAJ-NAK-CAP
2	D	501	KFD	CAI-CAJ-NAK-CAP
2	C	501	KFD	CAI-CAJ-NAK-CAL

Continued on next page...

Continued from previous page...

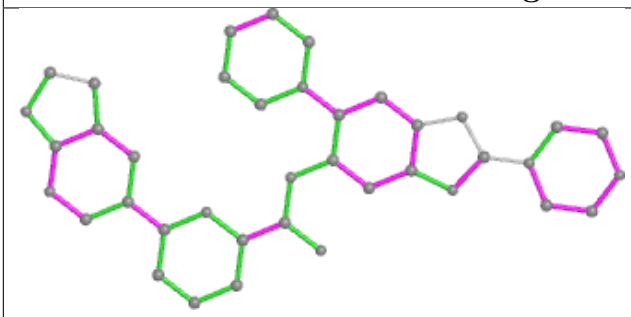
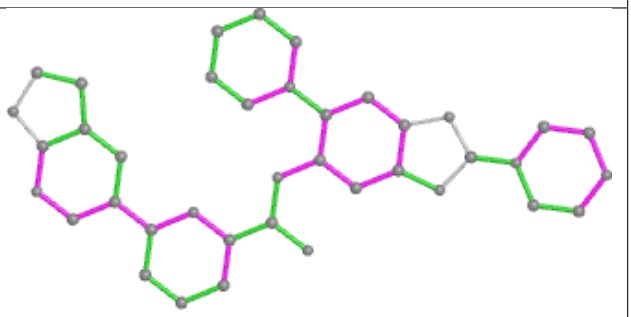
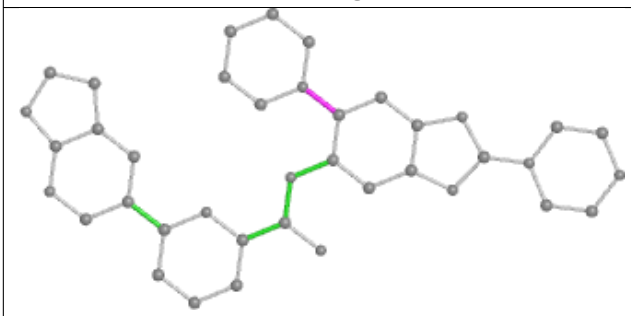
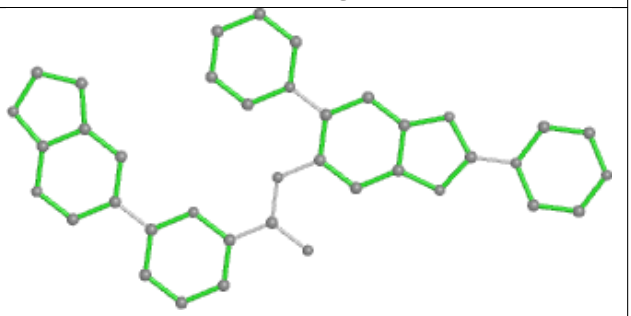
Mol	Chain	Res	Type	Atoms
2	A	501	KFD	CAI-CAJ-NAK-CAP
2	B	501	KFD	CAI-CAJ-NAK-CAL
2	D	501	KFD	CAI-CAJ-NAK-CAL
2	D	501	KFD	CAD-CAJ-NAK-CAP
2	A	501	KFD	CAD-CAJ-NAK-CAL
2	B	501	KFD	CAD-CAJ-NAK-CAP
2	C	501	KFD	CAD-CAJ-NAK-CAP

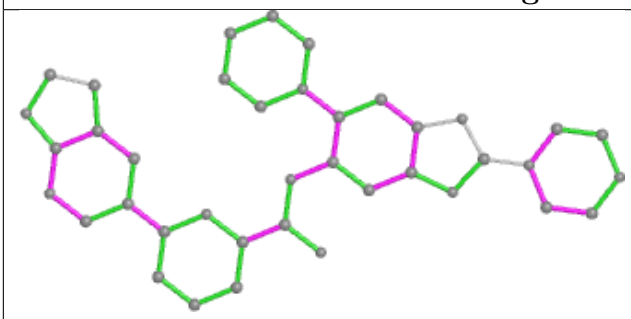
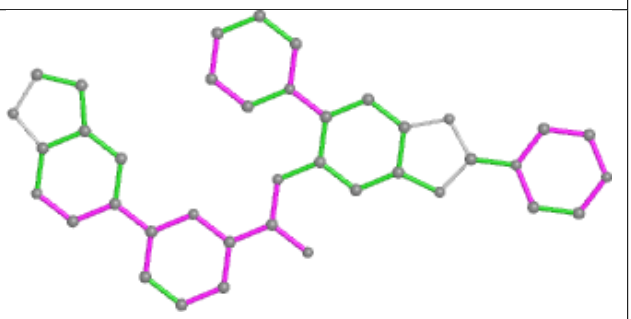
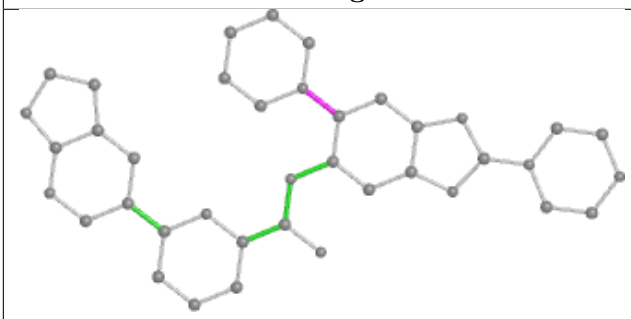
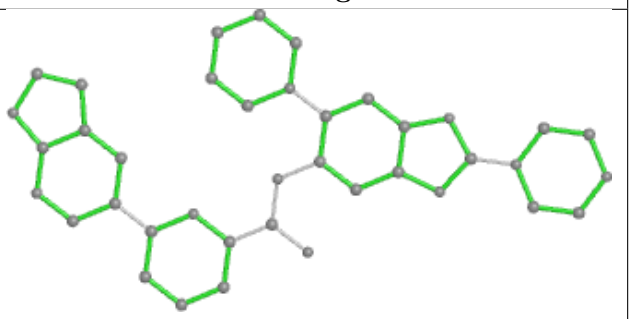
There are no ring outliers.

1 monomer is involved in 1 short contact:

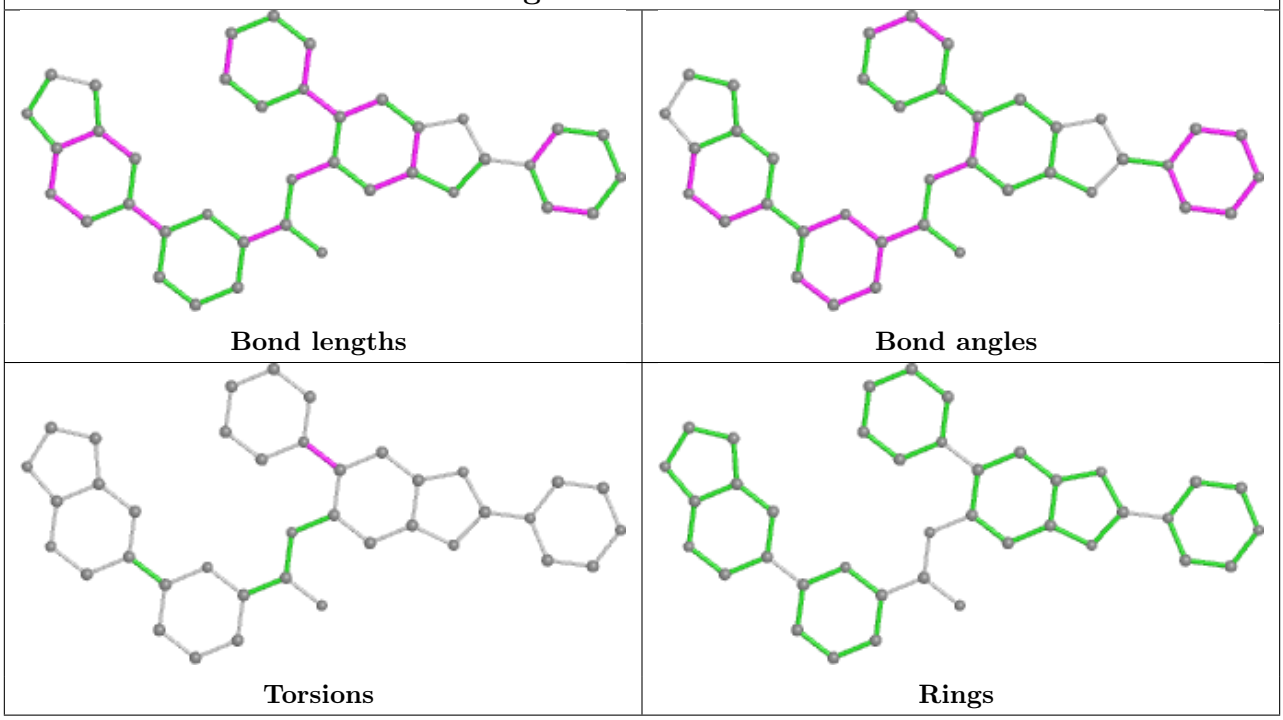
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	KFD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

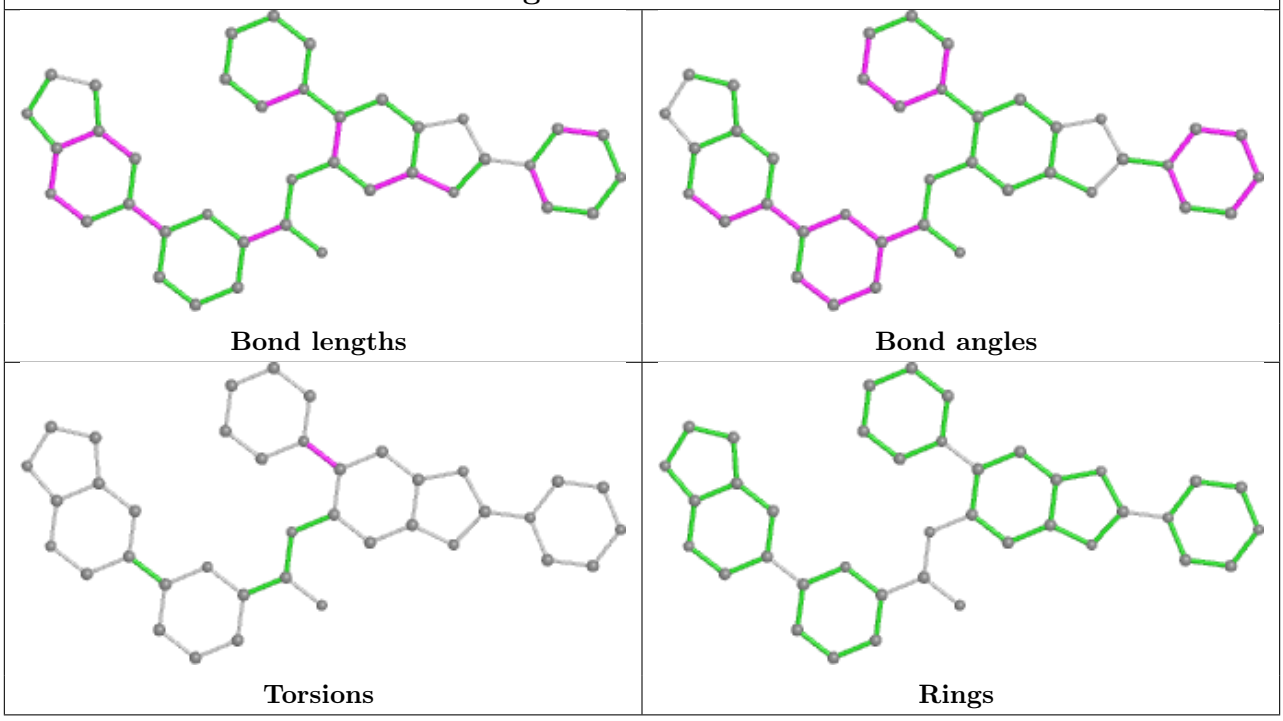
Ligand KFD B 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KFD D 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand KFD C 501



Ligand KFD A 501



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	285/297 (95%)	0.01	13 (4%)	32	31	29, 43, 80, 107	0
1	B	283/297 (95%)	0.21	19 (6%)	17	17	29, 50, 94, 114	0
1	C	286/297 (96%)	-0.07	9 (3%)	49	48	29, 43, 79, 103	0
1	D	277/297 (93%)	0.06	14 (5%)	28	27	30, 49, 93, 114	0
All	All	1131/1188 (95%)	0.05	55 (4%)	29	28	29, 45, 88, 114	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	197	PHE	6.9
1	B	197	PHE	6.0
1	D	228	GLN	5.3
1	D	196	GLY	4.4
1	D	215	LEU	4.3
1	D	258	LEU	4.0
1	C	221	ILE	3.9
1	B	216	ALA	3.8
1	A	256	ASP	3.8
1	B	256	ASP	3.7
1	B	226	LEU	3.7
1	B	196	GLY	3.6
1	C	256	ASP	3.6
1	A	223	THR	3.6
1	B	225	GLU	3.6
1	B	222	THR	3.5
1	A	343	VAL	3.4
1	D	230	PHE	3.4
1	A	222	THR	3.4
1	C	195	GLY	3.3
1	D	336	SER	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	187	VAL	3.3
1	B	459	ALA	3.2
1	B	223	THR	3.0
1	A	255	GLY	3.0
1	A	197	PHE	2.9
1	B	207	ASN	2.9
1	D	229	GLN	2.9
1	A	196	GLY	2.8
1	A	225	GLU	2.8
1	A	216	ALA	2.7
1	B	187	VAL	2.7
1	C	196	GLY	2.7
1	D	251	PHE	2.7
1	C	220	ASP	2.6
1	B	253	SER	2.6
1	B	230	PHE	2.6
1	D	254	ASP	2.6
1	A	224	GLU	2.5
1	D	335	ALA	2.5
1	D	188	GLY	2.4
1	C	216	ALA	2.4
1	B	224	GLU	2.3
1	A	226	LEU	2.3
1	B	287[A]	MET	2.3
1	A	336	SER	2.3
1	A	221	ILE	2.2
1	C	321[A]	GLU	2.1
1	B	186	SER	2.1
1	B	257	ASP	2.1
1	C	222	THR	2.1
1	B	228	GLN	2.1
1	B	406	GLU	2.0
1	C	223	THR	2.0
1	D	183	ARG	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	TPO	A	342	11/12	0.62	0.42	64,84,92,99	0
1	SEP	D	346	10/11	0.64	0.23	81,99,131,140	0
1	TPO	B	342	11/12	0.65	0.23	83,91,122,122	0
1	TPO	D	342	11/12	0.68	0.26	88,103,115,128	0
1	SEP	B	346	10/11	0.77	0.19	68,88,123,128	0
1	TPO	C	342	11/12	0.82	0.29	88,114,117,119	0
1	SEP	A	346	10/11	0.83	0.26	76,82,111,122	0
1	SEP	C	346	10/11	0.89	0.13	65,84,104,112	0
1	TPO	A	345	11/12	0.92	0.18	61,66,84,88	0
1	TPO	D	345	11/12	0.93	0.17	57,68,84,101	0
1	TPO	C	345	11/12	0.94	0.12	55,61,75,76	0
1	TPO	B	345	11/12	0.95	0.12	56,61,76,80	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

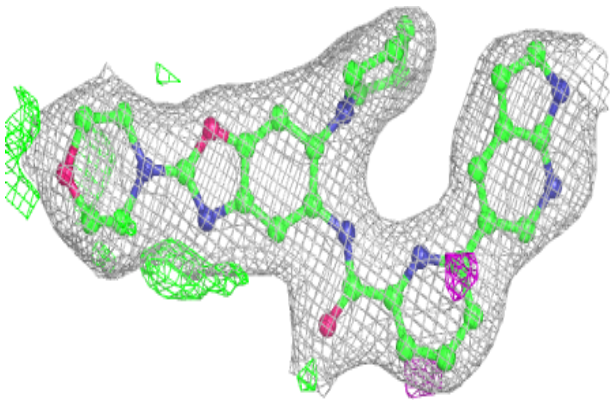
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

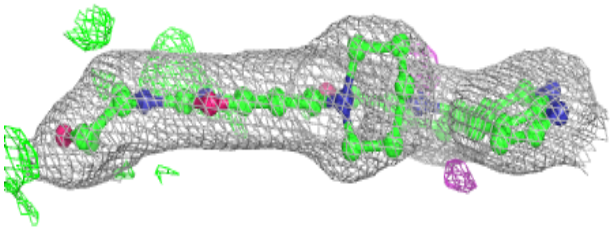
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	KFD	D	501	39/39	0.95	0.10	34,47,63,69	0
2	KFD	B	501	39/39	0.96	0.10	30,38,55,60	0
2	KFD	A	501	39/39	0.96	0.12	27,35,47,52	0
2	KFD	C	501	39/39	0.97	0.11	28,32,46,50	0

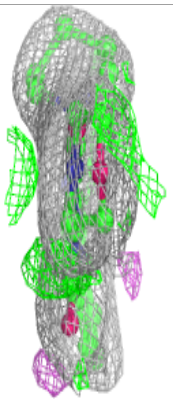
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around KFD D 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

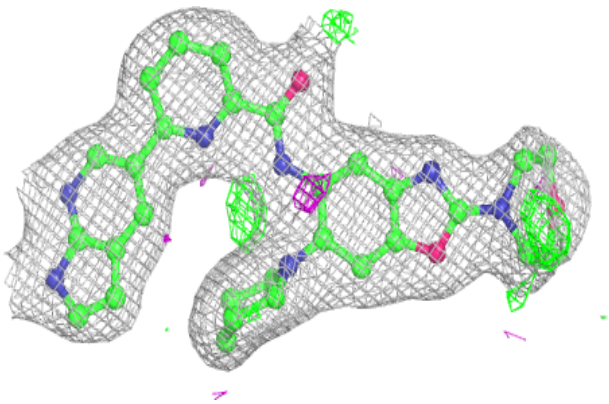


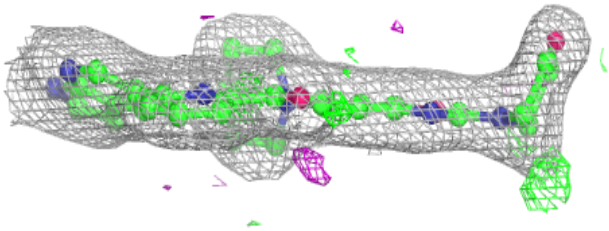


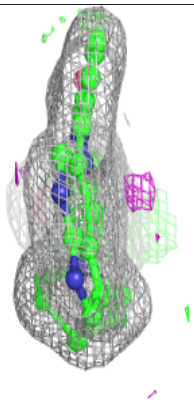


Electron density around KFD B 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

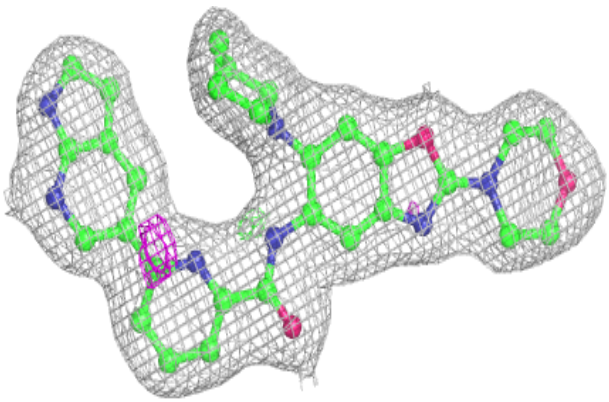


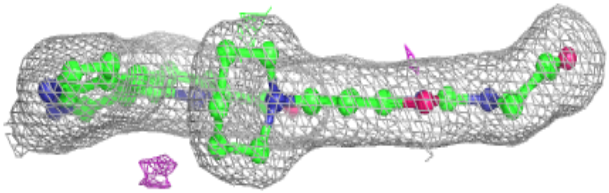


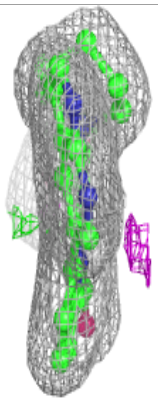


Electron density around KFD A 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

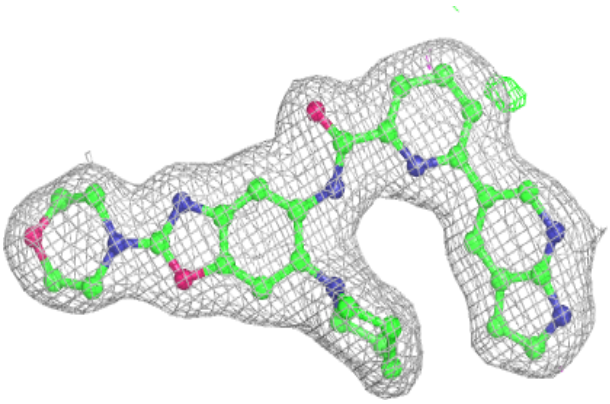


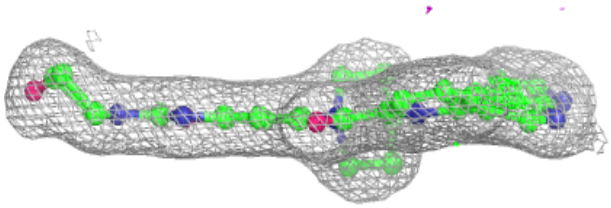


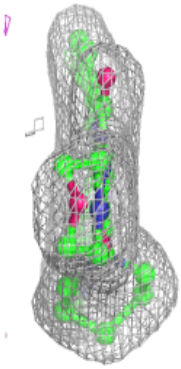


Electron density around KFD C 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.