Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2023 – 12:33 PM JST

PDB ID	:	5D7V
Title	:	Crystal structure of PTK6 kinase domain
Authors	:	Thakur, M.K.; Birudukota, S.; Swaminathan, S.; Tyagi, R.; Gosu, R.
Deposited on	:	2015-08-14
Resolution	:	2.33 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:

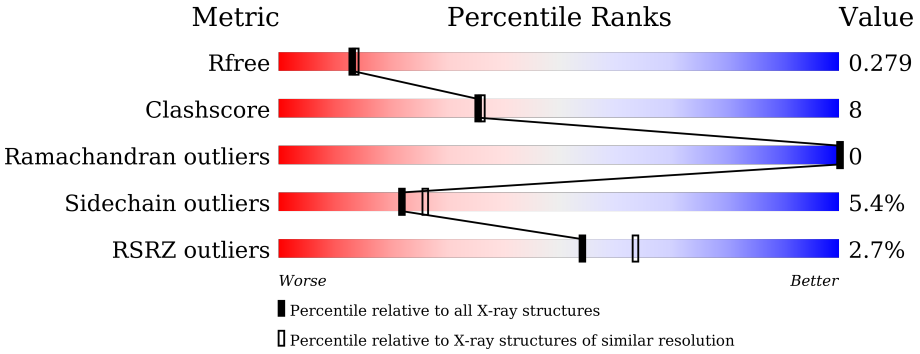
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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	269	2% 81% 15% •
1	B	269	% 79% 18% ••
1	C	269	4% 83% 14% ••
1	D	269	4% 83% 13% ••

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9141 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 Protein-tyrosine kinase 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	269	2214	1410	390	397	17	0	5	0
1	B	265	2161	1379	379	386	17	0	4	0
1	C	265	2165	1380	378	389	18	0	4	0
1	D	265	2143	1366	373	387	17	0	1	0

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	184	CXM	-	expression tag	UNP Q13882
A	433	THR	CYS	engineered mutation	UNP Q13882
A	447	HIS	-	expression tag	UNP Q13882
A	448	HIS	-	expression tag	UNP Q13882
A	449	HIS	-	expression tag	UNP Q13882
A	450	HIS	-	expression tag	UNP Q13882
A	451	HIS	-	expression tag	UNP Q13882
A	452	HIS	-	expression tag	UNP Q13882
B	184	CXM	-	expression tag	UNP Q13882
B	433	THR	CYS	engineered mutation	UNP Q13882
B	447	HIS	-	expression tag	UNP Q13882
B	448	HIS	-	expression tag	UNP Q13882
B	449	HIS	-	expression tag	UNP Q13882
B	450	HIS	-	expression tag	UNP Q13882
B	451	HIS	-	expression tag	UNP Q13882
B	452	HIS	-	expression tag	UNP Q13882
C	184	CXM	-	expression tag	UNP Q13882
C	433	THR	CYS	engineered mutation	UNP Q13882
C	447	HIS	-	expression tag	UNP Q13882
C	448	HIS	-	expression tag	UNP Q13882
C	449	HIS	-	expression tag	UNP Q13882

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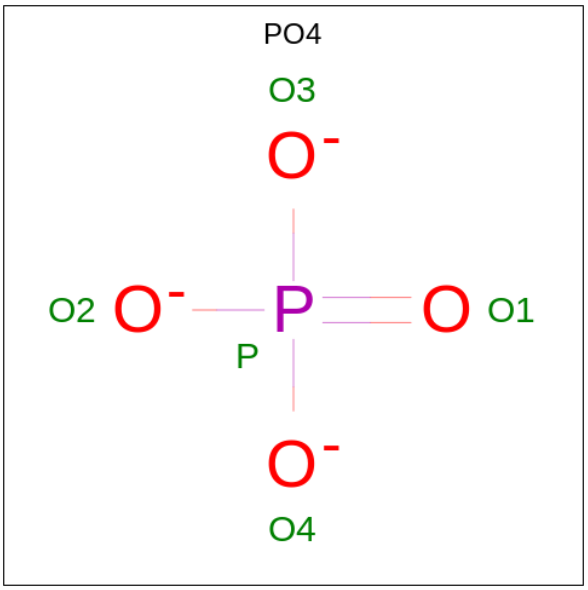
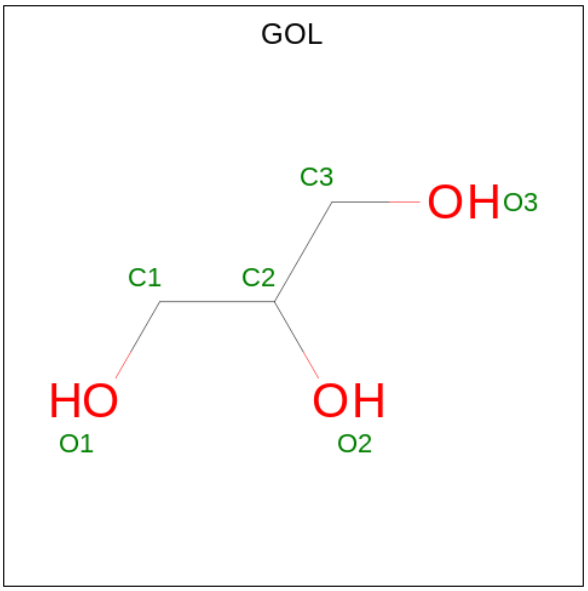
Chain	Residue	Modelled	Actual	Comment	Reference
C	450	HIS	-	expression tag	UNP Q13882
C	451	HIS	-	expression tag	UNP Q13882
C	452	HIS	-	expression tag	UNP Q13882
D	184	CXM	-	expression tag	UNP Q13882
D	433	THR	CYS	engineered mutation	UNP Q13882
D	447	HIS	-	expression tag	UNP Q13882
D	448	HIS	-	expression tag	UNP Q13882
D	449	HIS	-	expression tag	UNP Q13882
D	450	HIS	-	expression tag	UNP Q13882
D	451	HIS	-	expression tag	UNP Q13882
D	452	HIS	-	expression tag	UNP Q13882

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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



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

- Molecule 4 is water.

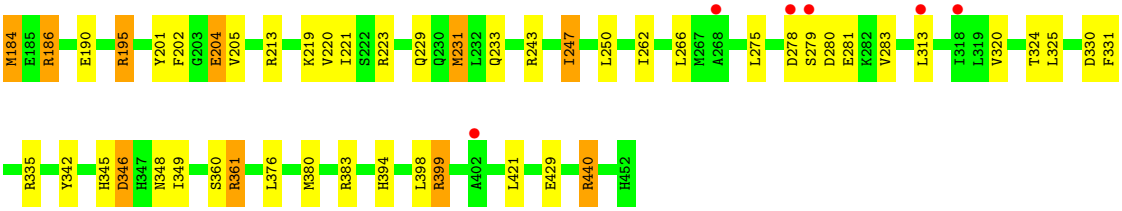
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	121	121	121	0	0
			Total	O		
4	B	78	78	78	0	0
			Total	O		
4	C	84	84	84	0	0
			Total	O		
4	D	83	83	83	0	0

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.

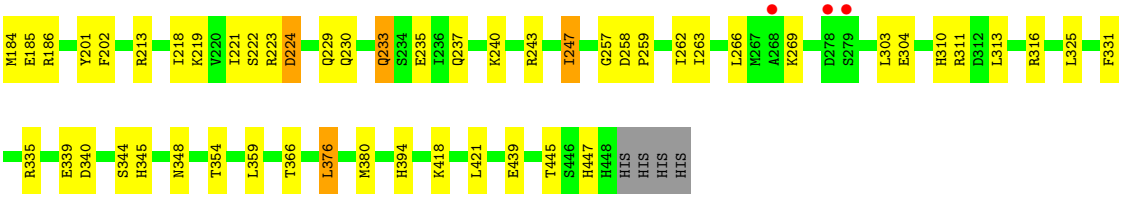
• Molecule 1: Protein-tyrosine kinase 6

Chain A:



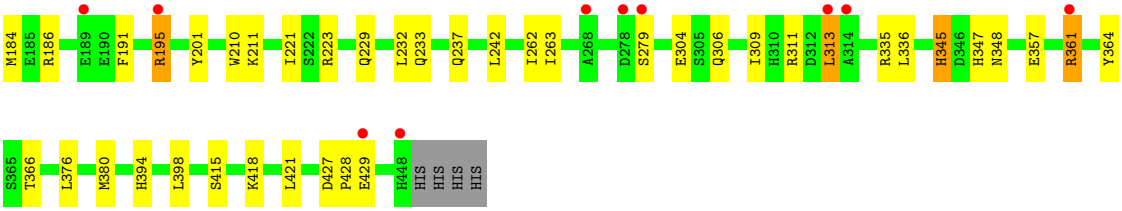
• Molecule 1: Protein-tyrosine kinase 6

Chain B:



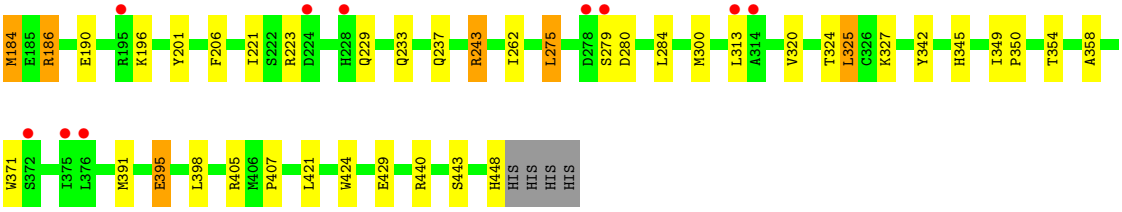
• Molecule 1: Protein-tyrosine kinase 6

Chain C:



• Molecule 1: Protein-tyrosine kinase 6

Chain D:


M184
E185
R186
E190
R195
K196
Y201
F206
I221
S222
R223
D224
H228
Q229
Q233
Q237
R243
I262
L275
D278
S279
D280
L284
M300
L313
A314
V320
T324
L325
C326
K327
Y342
H345
I349
P350
T354
A358
W371
S372
I375
L376
M391
E395
L398
R405
M406
P407
L421
W424
E429
R440
S443
H448
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	49.72Å 76.31Å 87.27Å 81.46° 75.92° 74.93°	Depositor
Resolution (Å)	50.00 – 2.33 29.10 – 2.33	Depositor EDS
% Data completeness (in resolution range)	96.0 (50.00-2.33) 96.0 (29.10-2.33)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.08 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.219 , 0.282 0.218 , 0.279	Depositor DCC
R_{free} test set	2476 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	27.2	Xtriage
Anisotropy	0.337	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 34.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9141	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.98% 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: CXM, GOL, PO4

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	0.43	0/2265	0.63	0/3065
1	B	0.41	0/2205	0.58	0/2984
1	C	0.39	0/2209	0.59	0/2989
1	D	0.39	0/2177	0.59	1/2947 (0.0%)
All	All	0.41	0/8856	0.60	1/11985 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	275	LEU	CA-CB-CG	5.75	128.53	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2214	0	2187	43	0
1	B	2161	0	2149	38	0
1	C	2165	0	2152	37	0
1	D	2143	0	2123	27	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	18	0	24	0	0
3	B	18	0	24	3	0
3	C	18	0	24	6	0
3	D	18	0	24	3	0
4	A	121	0	0	2	0
4	B	78	0	0	3	0
4	C	84	0	0	0	0
4	D	83	0	0	2	0
All	All	9141	0	8707	141	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 8.

All (141) 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:399:ARG:HG2	1:A:399:ARG:HH11	1.20	1.06
1:A:440:ARG:HH11	1:A:440:ARG:HG3	1.22	1.05
1:C:361:ARG:HG3	1:C:361:ARG:HH21	1.26	0.98
1:A:348:ASN:HD22	1:A:394[B]:HIS:HE1	1.07	0.93
1:A:348:ASN:HD22	1:A:394[B]:HIS:CE1	1.92	0.86
1:C:223:ARG:NH2	1:C:229:GLN:OE1	2.07	0.86
1:B:348:ASN:HD22	1:B:394[B]:HIS:HE1	1.23	0.85
1:C:361:ARG:HG3	1:C:361:ARG:NH2	1.88	0.84
1:C:311:ARG:HH11	3:C:503:GOL:H11	1.43	0.83
1:A:195:ARG:CG	1:A:195:ARG:HH11	1.91	0.82
1:B:316:ARG:NH2	3:B:502:GOL:O1	2.11	0.82
1:A:348:ASN:ND2	1:A:394[B]:HIS:HE1	1.78	0.82
1:A:223:ARG:NH2	1:A:229:GLN:OE1	2.14	0.81
1:A:440:ARG:HG3	1:A:440:ARG:NH1	1.94	0.79
1:C:348:ASN:ND2	1:C:394[B]:HIS:HE1	1.80	0.78
1:D:221:ILE:HD12	1:D:262:ILE:HD12	1.67	0.77
1:B:213:ARG:HD3	1:D:407:PRO:HB3	1.68	0.73
1:A:195:ARG:HH11	1:A:195:ARG:HG2	1.53	0.72
1:A:376:LEU:HD22	1:A:380:MET:CE	2.19	0.72
1:B:348:ASN:HD22	1:B:394[B]:HIS:CE1	2.05	0.72
1:A:376:LEU:HD22	1:A:380:MET:HE2	1.72	0.70
1:C:376:LEU:HD23	1:C:380:MET:HE3	1.73	0.70
1:C:376:LEU:CD2	1:C:380:MET:CE	2.69	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:ARG:HE	3:C:504:GOL:H12	1.55	0.69
1:A:361:ARG:HH12	1:B:439[A]:GLU:CD	1.96	0.69
1:C:361:ARG:HH21	1:C:361:ARG:CG	2.03	0.68
1:C:376:LEU:HD23	1:C:380:MET:CE	2.24	0.68
1:A:399:ARG:HH11	1:A:399:ARG:CG	2.04	0.67
1:C:415:SER:HA	1:C:418:LYS:HE3	1.75	0.67
1:C:376:LEU:CD2	1:C:380:MET:HE3	2.24	0.67
1:A:399:ARG:HG2	1:A:399:ARG:NH1	2.00	0.67
1:A:348:ASN:ND2	1:A:394[B]:HIS:CE1	2.58	0.66
1:C:348:ASN:ND2	1:C:394[B]:HIS:CE1	2.64	0.65
1:B:348:ASN:ND2	1:B:394[B]:HIS:HE1	1.93	0.64
1:B:221:ILE:HD12	1:B:262:ILE:HD12	1.81	0.62
1:B:348:ASN:ND2	1:B:394[B]:HIS:CE1	2.66	0.61
1:A:204[A]:GLU:HG2	1:A:220:VAL:HB	1.83	0.61
1:D:186:ARG:HG3	1:D:190:GLU:OE1	2.02	0.60
1:A:275:LEU:HD21	1:A:320:VAL:HG21	1.83	0.59
1:D:243:ARG:NH1	4:D:601:HOH:O	2.36	0.59
1:C:233:GLN:O	1:C:237:GLN:HG2	2.05	0.57
1:A:186:ARG:HG3	1:A:190:GLU:OE1	2.05	0.57
1:C:376:LEU:CD2	1:C:380:MET:HE2	2.34	0.56
1:D:275:LEU:O	1:D:279:SER:HB3	2.06	0.56
1:A:195:ARG:HG2	1:A:195:ARG:NH1	2.20	0.56
1:A:201:TYR:HB3	1:A:345:HIS:CG	2.43	0.54
1:A:202:PHE:CZ	1:A:205:VAL:HG22	2.43	0.54
1:A:342:TYR:O	1:A:345:HIS:HD2	1.91	0.54
1:B:185:GLU:HG2	4:B:601:HOH:O	2.06	0.54
1:B:304:GLU:HG3	1:B:366:THR:HG21	1.90	0.54
1:C:195:ARG:HH11	1:C:195:ARG:CG	2.23	0.52
1:C:376:LEU:HD21	1:C:380:MET:HE2	1.92	0.52
1:B:233:GLN:NE2	4:B:601:HOH:O	2.43	0.52
1:A:313:LEU:HD22	1:A:376:LEU:HD12	1.92	0.52
1:D:275:LEU:HD21	1:D:320:VAL:HG11	1.91	0.52
1:C:357:GLU:O	1:C:361:ARG:HB2	2.09	0.51
1:B:223:ARG:NH2	1:B:229:GLN:OE1	2.44	0.50
1:C:348:ASN:HD22	1:C:394[B]:HIS:CE1	2.29	0.50
1:D:354:THR:HG22	1:D:358:ALA:HB3	1.94	0.50
1:B:376:LEU:HD22	1:B:380:MET:HE2	1.94	0.50
1:B:258:ASP:OD1	1:B:259:PRO:HA	2.11	0.50
1:A:279:SER:O	1:A:280:ASP:OD1	2.30	0.50
1:B:201:TYR:HB3	1:B:345:HIS:CG	2.47	0.50
1:C:309:ILE:O	3:C:504:GOL:H11	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:GLN:NE2	4:A:605:HOH:O	2.45	0.49
1:B:237:GLN:NE2	1:B:240:LYS:HE2	2.27	0.49
1:D:196:LYS:HG2	1:D:206:PHE:CE2	2.48	0.49
1:B:376:LEU:HD22	1:B:380:MET:CE	2.43	0.49
1:D:233:GLN:O	1:D:237:GLN:HG2	2.11	0.49
1:D:201:TYR:HB3	1:D:345:HIS:CG	2.48	0.49
1:C:376:LEU:HD21	1:C:380:MET:CE	2.41	0.48
1:A:186:ARG:CG	1:A:190:GLU:OE1	2.61	0.48
1:A:221:ILE:HD12	1:A:262:ILE:HD13	1.95	0.48
1:A:376:LEU:HD22	1:A:380:MET:HE3	1.91	0.48
1:B:223:ARG:NH1	1:B:257:GLY:O	2.45	0.48
1:B:310:HIS:O	1:B:311:ARG:HB2	2.14	0.48
1:C:304:GLU:HG3	1:C:366:THR:HG21	1.96	0.48
1:D:345:HIS:CE1	3:D:502:GOL:H32	2.48	0.48
1:A:231:MET:HG3	4:A:667:HOH:O	2.14	0.47
1:D:196:LYS:HB3	1:D:196:LYS:NZ	2.30	0.47
1:D:345:HIS:HE1	3:D:502:GOL:H32	1.79	0.47
1:B:313:LEU:HD22	1:B:376:LEU:HD12	1.97	0.47
1:B:224:ASP:OD1	1:B:224:ASP:N	2.45	0.47
1:A:440:ARG:HH11	1:A:440:ARG:CG	2.07	0.47
1:D:186:ARG:CG	1:D:190:GLU:OE1	2.62	0.47
1:B:340:ASP:HB3	1:C:347:HIS:HB3	1.97	0.47
1:D:440:ARG:HA	1:D:440:ARG:HD2	1.79	0.47
1:C:221:ILE:HD12	1:C:262:ILE:HD12	1.97	0.46
1:B:213:ARG:NH2	1:D:405:ARG:O	2.49	0.46
1:D:221:ILE:CD1	1:D:262:ILE:HD12	2.42	0.46
1:D:443:SER:HA	1:D:448:HIS:CD2	2.51	0.46
1:C:232:LEU:HD12	1:C:336:LEU:HD22	1.99	0.45
1:A:376:LEU:CD2	1:A:380:MET:HE2	2.45	0.44
1:C:376:LEU:HD23	1:C:380:MET:HE2	1.98	0.44
1:D:279:SER:HB2	1:D:284:LEU:HB3	2.00	0.44
1:A:195:ARG:CG	1:A:195:ARG:NH1	2.62	0.44
1:C:210:TRP:CE2	1:C:211:LYS:HG3	2.53	0.44
1:D:184[B]:CXM:HA	1:D:184[B]:CXM:CE	2.48	0.44
1:B:316:ARG:NH2	3:B:502:GOL:HO1	2.14	0.44
1:B:354:THR:HB	1:B:359:LEU:HD11	2.00	0.43
1:C:311:ARG:NH1	3:C:503:GOL:H11	2.22	0.43
1:B:218:ILE:HG12	1:B:263:ILE:HG12	2.00	0.43
1:C:348:ASN:HD22	1:C:394[B]:HIS:HE1	1.58	0.43
1:A:219:LYS:HE2	1:A:330:ASP:OD2	2.18	0.43
1:D:300:MET:HG3	1:D:313:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184[B]:CXM:ON2	1:A:250:LEU:HD22	2.19	0.43
1:B:247:ILE:HD11	1:B:303:LEU:HG	2.00	0.43
1:D:223:ARG:NH2	1:D:229:GLN:OE1	2.50	0.43
1:B:344:SER:HA	1:B:348:ASN:OD1	2.18	0.43
1:D:391:MET:HB3	1:D:395:GLU:HG2	1.99	0.43
1:D:325:LEU:HD21	1:D:327:LYS:HE2	2.00	0.43
1:A:195:ARG:HH11	1:A:195:ARG:HG3	1.74	0.43
1:C:364:TYR:CZ	3:C:503:GOL:H12	2.54	0.43
1:B:344:SER:HB3	1:C:348:ASN:ND2	2.34	0.42
1:C:191:PHE:CE2	1:C:263:ILE:HD13	2.53	0.42
1:D:371:TRP:CE3	1:D:424:TRP:HA	2.55	0.42
1:B:339:GLU:HG3	3:B:504:GOL:H2	2.02	0.42
1:A:280:ASP:HB3	1:A:281[A]:GLU:H	1.76	0.42
1:A:279:SER:HB2	1:A:283:VAL:HB	2.02	0.42
1:B:202:PHE:CZ	1:B:219:LYS:HE3	2.55	0.42
1:B:335:ARG:NH1	4:B:608:HOH:O	2.53	0.42
1:B:445:THR:OG1	1:B:447:HIS:O	2.30	0.42
1:D:349:ILE:N	1:D:350:PRO:CD	2.83	0.41
3:D:502:GOL:H31	4:D:654:HOH:O	2.20	0.41
1:A:346:ASP:HB2	1:A:349:ILE:HG22	2.02	0.41
1:B:235:GLU:OE1	1:B:335:ARG:NH1	2.54	0.41
1:C:311:ARG:NE	3:C:504:GOL:H12	2.29	0.41
1:B:202:PHE:O	1:B:221:ILE:HG23	2.20	0.41
1:B:243:ARG:HB2	1:B:243:ARG:NH1	2.36	0.41
1:A:360:SER:HB3	1:A:361:ARG:HE	1.85	0.41
1:B:237:GLN:HE22	1:B:240:LYS:HE2	1.86	0.41
1:D:342:TYR:O	1:D:345:HIS:HD2	2.02	0.41
1:A:247:ILE:HG23	1:A:331:PHE:CE1	2.56	0.41
1:B:247:ILE:HG23	1:B:331:PHE:CE1	2.55	0.41
1:C:313:LEU:HD22	1:C:376:LEU:CD1	2.51	0.41
1:A:202:PHE:CE2	1:A:205:VAL:HG22	2.56	0.41
1:C:427:ASP:HA	1:C:428:PRO:HD2	1.91	0.41
1:A:202:PHE:HZ	1:A:205:VAL:HG22	1.85	0.40
1:C:201:TYR:HB3	1:C:345:HIS:CG	2.57	0.40
1:C:242:LEU:CD2	1:C:306:GLN:HG2	2.51	0.40
1:A:280:ASP:OD1	1:A:383:ARG:HD3	2.21	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	271/269 (101%)	263 (97%)	8 (3%)	0	100	100
1	B	266/269 (99%)	257 (97%)	9 (3%)	0	100	100
1	C	266/269 (99%)	259 (97%)	7 (3%)	0	100	100
1	D	263/269 (98%)	254 (97%)	9 (3%)	0	100	100
All	All	1066/1076 (99%)	1033 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	241/238 (101%)	221 (92%)	20 (8%)	11	11
1	B	234/238 (98%)	222 (95%)	12 (5%)	24	29
1	C	236/238 (99%)	226 (96%)	10 (4%)	30	37
1	D	232/238 (98%)	223 (96%)	9 (4%)	32	41
All	All	943/952 (99%)	892 (95%)	51 (5%)	22	26

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	186	ARG
1	A	195	ARG

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Mol	Chain	Res	Type
1	A	204[A]	GLU
1	A	204[B]	GLU
1	A	213	ARG
1	A	231	MET
1	A	243	ARG
1	A	247	ILE
1	A	266	LEU
1	A	278	ASP
1	A	324	THR
1	A	325	LEU
1	A	335	ARG
1	A	346	ASP
1	A	361	ARG
1	A	398	LEU
1	A	399	ARG
1	A	421	LEU
1	A	429	GLU
1	A	440	ARG
1	B	186	ARG
1	B	222	SER
1	B	224	ASP
1	B	230	GLN
1	B	233	GLN
1	B	247	ILE
1	B	266	LEU
1	B	269	LYS
1	B	325	LEU
1	B	376	LEU
1	B	418	LYS
1	B	421	LEU
1	C	186	ARG
1	C	195	ARG
1	C	279	SER
1	C	313	LEU
1	C	335	ARG
1	C	345	HIS
1	C	361	ARG
1	C	398	LEU
1	C	421	LEU
1	C	429	GLU
1	D	186	ARG
1	D	243	ARG

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Mol	Chain	Res	Type
1	D	280	ASP
1	D	324	THR
1	D	325	LEU
1	D	395	GLU
1	D	398	LEU
1	D	421	LEU
1	D	429	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	317	ASN
1	A	345	HIS
1	A	348	ASN
1	B	233	GLN
1	B	237	GLN
1	B	317	ASN
1	B	345	HIS
1	C	317	ASN
1	C	347	HIS
1	C	348	ASN
1	D	233	GLN
1	D	317	ASN
1	D	345	HIS
1	D	430	GLN
1	D	448	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

8 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	CXM	C	184[A]	-	8,10,11	0.79	0	7,11,13	1.59	1 (14%)
1	CXM	A	184[B]	-	8,10,11	0.81	0	7,11,13	1.33	1 (14%)
1	CXM	D	184[A]	-	8,10,11	0.74	0	7,11,13	1.60	2 (28%)
1	CXM	B	184[A]	-	8,10,11	0.77	0	7,11,13	1.33	1 (14%)
1	CXM	C	184[B]	-	8,10,11	0.75	0	7,11,13	1.48	1 (14%)
1	CXM	D	184[B]	-	8,10,11	0.78	0	7,11,13	1.73	2 (28%)
1	CXM	B	184[B]	-	8,10,11	0.76	0	7,11,13	1.41	1 (14%)
1	CXM	A	184[A]	-	8,10,11	0.72	0	7,11,13	1.24	1 (14%)

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	CXM	C	184[A]	-	-	4/9/10/12	-
1	CXM	A	184[B]	-	-	3/9/10/12	-
1	CXM	D	184[A]	-	-	4/9/10/12	-
1	CXM	B	184[A]	-	-	2/9/10/12	-
1	CXM	C	184[B]	-	-	6/9/10/12	-
1	CXM	D	184[B]	-	-	6/9/10/12	-
1	CXM	B	184[B]	-	-	6/9/10/12	-
1	CXM	A	184[A]	-	-	4/9/10/12	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	184[A]	CXM	ON1-CN-N	-3.53	119.06	124.85
1	D	184[B]	CXM	ON1-CN-N	-3.39	119.29	124.85
1	C	184[B]	CXM	ON1-CN-N	-3.38	119.30	124.85
1	D	184[A]	CXM	ON1-CN-N	-3.38	119.31	124.85
1	B	184[A]	CXM	ON1-CN-N	-2.74	120.35	124.85
1	B	184[B]	CXM	ON1-CN-N	-2.65	120.49	124.85
1	A	184[A]	CXM	ON1-CN-N	-2.51	120.74	124.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	184[B]	CXM	ON1-CN-N	-2.47	120.79	124.85
1	D	184[B]	CXM	C-CA-N	2.19	113.68	109.73
1	D	184[A]	CXM	C-CA-N	2.17	113.66	109.73

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	184[A]	CXM	N-CA-CB-CG
1	B	184[A]	CXM	N-CA-CB-CG
1	B	184[B]	CXM	C-CA-CB-CG
1	C	184[A]	CXM	ON2-CN-N-CA
1	C	184[A]	CXM	N-CA-CB-CG
1	C	184[B]	CXM	N-CA-CB-CG
1	C	184[B]	CXM	C-CA-CB-CG
1	D	184[A]	CXM	C-CA-N-CN
1	D	184[A]	CXM	ON2-CN-N-CA
1	D	184[A]	CXM	N-CA-CB-CG
1	D	184[B]	CXM	C-CA-N-CN
1	D	184[B]	CXM	ON1-CN-N-CA
1	D	184[B]	CXM	ON2-CN-N-CA
1	D	184[B]	CXM	C-CA-CB-CG
1	C	184[A]	CXM	ON1-CN-N-CA
1	D	184[A]	CXM	ON1-CN-N-CA
1	A	184[B]	CXM	CA-CB-CG-SD
1	D	184[B]	CXM	CA-CB-CG-SD
1	B	184[B]	CXM	N-CA-CB-CG
1	C	184[B]	CXM	CB-CG-SD-CE
1	B	184[B]	CXM	CA-CB-CG-SD
1	D	184[B]	CXM	N-CA-CB-CG
1	B	184[B]	CXM	CB-CG-SD-CE
1	A	184[A]	CXM	C-CA-N-CN
1	A	184[B]	CXM	C-CA-N-CN
1	B	184[A]	CXM	C-CA-N-CN
1	B	184[B]	CXM	C-CA-N-CN
1	A	184[A]	CXM	CB-CA-N-CN
1	A	184[B]	CXM	CB-CA-N-CN
1	B	184[B]	CXM	CB-CA-N-CN
1	C	184[B]	CXM	CB-CA-N-CN
1	A	184[A]	CXM	C-CA-CB-CG
1	C	184[A]	CXM	C-CA-CB-CG
1	C	184[B]	CXM	ON1-CN-N-CA

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Mol	Chain	Res	Type	Atoms
1	C	184[B]	CXM	C-CA-N-CN

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	184[B]	CXM	1	0
1	D	184[B]	CXM	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

16 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	$\#\|Z\| > 2$
3	GOL	D	503	-	5,5,5	0.39	0	5,5,5	0.73	0
2	PO4	D	501	-	4,4,4	0.85	0	6,6,6	0.50	0
2	PO4	A	501	-	4,4,4	0.81	0	6,6,6	0.46	0
3	GOL	A	504	-	5,5,5	0.34	0	5,5,5	0.45	0
2	PO4	C	501	-	4,4,4	0.81	0	6,6,6	0.45	0
3	GOL	B	503	-	5,5,5	0.38	0	5,5,5	0.21	0
3	GOL	B	504	-	5,5,5	0.37	0	5,5,5	0.28	0
3	GOL	A	503	-	5,5,5	0.35	0	5,5,5	0.25	0
3	GOL	C	502	-	5,5,5	0.36	0	5,5,5	0.39	0
3	GOL	C	503	-	5,5,5	0.36	0	5,5,5	0.38	0
3	GOL	C	504	-	5,5,5	0.39	0	5,5,5	0.37	0
3	GOL	D	502	-	5,5,5	0.32	0	5,5,5	0.56	0
3	GOL	B	502	-	5,5,5	0.30	0	5,5,5	0.66	0
3	GOL	A	502	-	5,5,5	0.45	0	5,5,5	0.30	0
3	GOL	D	504	-	5,5,5	0.35	0	5,5,5	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PO4	B	501	-	4,4,4	0.80	0	6,6,6	0.39	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	D	503	-	-	4/4/4/4	-
3	GOL	B	503	-	-	2/4/4/4	-
3	GOL	A	504	-	-	2/4/4/4	-
3	GOL	C	503	-	-	4/4/4/4	-
3	GOL	B	504	-	-	1/4/4/4	-
3	GOL	A	503	-	-	2/4/4/4	-
3	GOL	D	502	-	-	2/4/4/4	-
3	GOL	C	504	-	-	3/4/4/4	-
3	GOL	B	502	-	-	0/4/4/4	-
3	GOL	A	502	-	-	4/4/4/4	-
3	GOL	D	504	-	-	2/4/4/4	-
3	GOL	C	502	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	GOL	O1-C1-C2-C3
3	A	502	GOL	C1-C2-C3-O3
3	A	504	GOL	C1-C2-C3-O3
3	C	503	GOL	O1-C1-C2-C3
3	C	503	GOL	C1-C2-C3-O3
3	D	502	GOL	C1-C2-C3-O3
3	D	504	GOL	O1-C1-C2-C3
3	D	503	GOL	O1-C1-C2-O2
3	D	503	GOL	O2-C2-C3-O3
3	A	503	GOL	O1-C1-C2-C3
3	B	503	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	C	504	GOL	O1-C1-C2-C3
3	C	504	GOL	C1-C2-C3-O3
3	D	503	GOL	O1-C1-C2-C3
3	D	503	GOL	C1-C2-C3-O3
3	A	502	GOL	O2-C2-C3-O3
3	A	504	GOL	O2-C2-C3-O3
3	C	503	GOL	O1-C1-C2-O2
3	C	504	GOL	O2-C2-C3-O3
3	D	502	GOL	O2-C2-C3-O3
3	D	504	GOL	O1-C1-C2-O2
3	A	502	GOL	O1-C1-C2-O2
3	C	503	GOL	O2-C2-C3-O3
3	C	502	GOL	O1-C1-C2-O2
3	B	504	GOL	O1-C1-C2-C3
3	C	502	GOL	O1-C1-C2-C3
3	A	503	GOL	O1-C1-C2-O2
3	B	503	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	504	GOL	1	0
3	C	503	GOL	3	0
3	C	504	GOL	3	0
3	D	502	GOL	3	0
3	B	502	GOL	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	268/269 (99%)	0.20	6 (2%)	62	71	16, 24, 33, 40	0
1	B	264/269 (98%)	0.15	3 (1%)	80	86	16, 25, 33, 40	0
1	C	264/269 (98%)	0.34	10 (3%)	40	51	15, 26, 38, 43	0
1	D	264/269 (98%)	0.33	10 (3%)	40	51	20, 28, 40, 44	0
All	All	1060/1076 (98%)	0.25	29 (2%)	54	64	15, 26, 37, 44	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	278	ASP	3.9
1	A	268	ALA	3.8
1	A	278	ASP	3.6
1	C	268	ALA	3.6
1	C	278	ASP	3.2
1	C	361	ARG	2.9
1	B	279	SER	2.8
1	D	279	SER	2.7
1	D	376	LEU	2.7
1	C	195	ARG	2.7
1	A	279	SER	2.6
1	B	278	ASP	2.6
1	C	429	GLU	2.6
1	C	313	LEU	2.5
1	C	279	SER	2.4
1	D	375	ILE	2.4
1	D	195	ARG	2.4
1	B	268	ALA	2.3
1	A	318	ILE	2.3
1	A	313	LEU	2.3
1	D	313	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	228	HIS	2.2
1	C	189	GLU	2.1
1	D	314	ALA	2.1
1	D	224	ASP	2.1
1	A	402	ALA	2.0
1	C	314	ALA	2.0
1	C	448	HIS	2.0
1	D	372	SER	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	CXM	D	184[A]	11/12	0.90	0.17	26,29,29,29	8
1	CXM	D	184[B]	11/12	0.90	0.17	28,29,29,29	8
1	CXM	B	184[A]	11/12	0.91	0.16	25,25,25,26	8
1	CXM	B	184[B]	11/12	0.91	0.16	23,25,25,26	8
1	CXM	C	184[A]	11/12	0.94	0.15	30,32,32,32	8
1	CXM	C	184[B]	11/12	0.94	0.15	32,32,32,33	8
1	CXM	A	184[A]	11/12	0.96	0.13	17,20,20,21	8
1	CXM	A	184[B]	11/12	0.96	0.13	18,20,20,21	8

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	D	502	6/6	0.79	0.31	32,34,34,35	0
2	PO4	D	501	5/5	0.84	0.28	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PO4	A	501	5/5	0.84	0.29	66,66,66,66	0
2	PO4	C	501	5/5	0.86	0.38	71,71,71,72	0
3	GOL	A	503	6/6	0.87	0.16	33,34,35,35	0
3	GOL	D	504	6/6	0.87	0.22	34,34,35,35	0
2	PO4	B	501	5/5	0.88	0.29	60,61,61,61	0
3	GOL	D	503	6/6	0.88	0.17	31,33,34,35	0
3	GOL	C	504	6/6	0.88	0.18	40,41,41,41	0
3	GOL	A	504	6/6	0.91	0.16	37,38,38,38	0
3	GOL	C	503	6/6	0.91	0.17	37,39,39,40	0
3	GOL	A	502	6/6	0.91	0.22	35,36,36,37	0
3	GOL	B	504	6/6	0.92	0.14	34,35,35,35	0
3	GOL	C	502	6/6	0.95	0.19	25,26,26,26	0
3	GOL	B	503	6/6	0.95	0.11	29,29,30,30	0
3	GOL	B	502	6/6	0.96	0.18	20,22,24,25	0

6.5 Other polymers (i)

There are no such residues in this entry.