Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:58 AM GMT

PDB ID	:	2Z0P
Title	:	Crystal structure of PH domain of Bruton's tyrosine kinase
Authors	:	Murayama, K.; Kato-Murayama, M.; Mishima, C.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2007-05-07
Resolution	:	2.58 Å(reported)

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

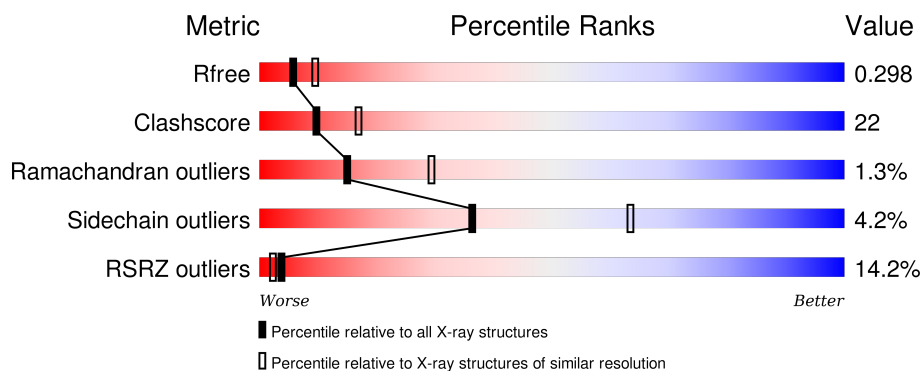|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.58 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	Percentile Ranks	Value
Rfree		0.298
Clashscore		22
Ramachandran outliers		1.3%
Sidechain outliers		4.2%
RSRZ outliers		14.2%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2636 (2.60-2.56)
Clashscore	102246	3003 (2.60-2.56)
Ramachandran outliers	100387	2956 (2.60-2.56)
Sidechain outliers	100360	2956 (2.60-2.56)
RSRZ outliers	91569	2642 (2.60-2.56)

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 <=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	169	15% — 49% 41% · 7%
1	B	169	12% — 62% 31% ·· 5%
1	C	169	17% — 49% 39% ·· 8%
1	D	169	9% — 64% 29% · 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	4PT	B	502	X	-	-	-
3	4PT	D	504	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5510 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.
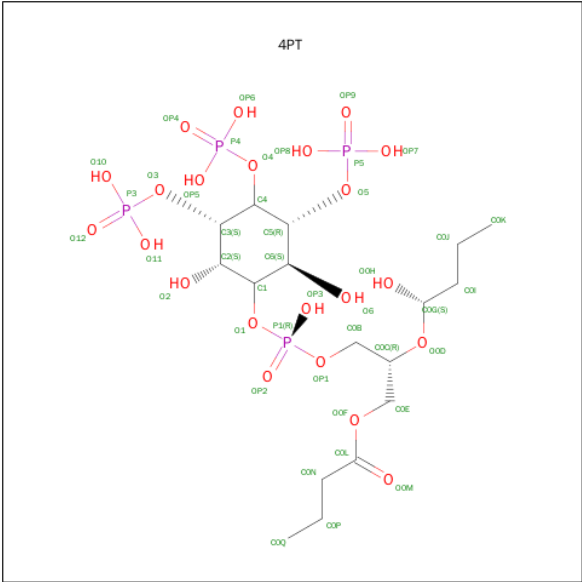
- Molecule 1 is a protein called Tyrosine-protein kinase BTK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	0	0	0
			1316	851	226	232	7			
1	B	161	Total	C	N	O	S	0	0	0
			1343	865	230	241	7			
1	C	155	Total	C	N	O	S	0	0	0
			1296	836	222	231	7			
1	D	161	Total	C	N	O	S	0	0	0
			1341	865	230	239	7			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		
2	A	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

- Molecule 3 is (2R)-3-{[(S)-{[(2S,3R,5S,6S)-2,6-DIHYDROXY-3,4,5-TRIS(PHOSPHONOO XY)CYCLOHEXYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-2-(1-HYDROXYBUTOX Y)PROPYL BUTYRATE (three-letter code: 4PT) (formula: $C_{17}H_{36}O_{22}P_4$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 28	C 6	O 18	P 4	0	0
3	B	1	Total 43	C 17	O 22	P 4	0	0
3	C	1	Total 28	C 6	O 18	P 4	0	0
3	D	1	Total 43	C 17	O 22	P 4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	13	Total 13	O 13	0	0
4	B	25	Total 25	O 25	0	0
4	C	6	Total 6	O 6	0	0
4	D	24	Total 24	O 24	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 on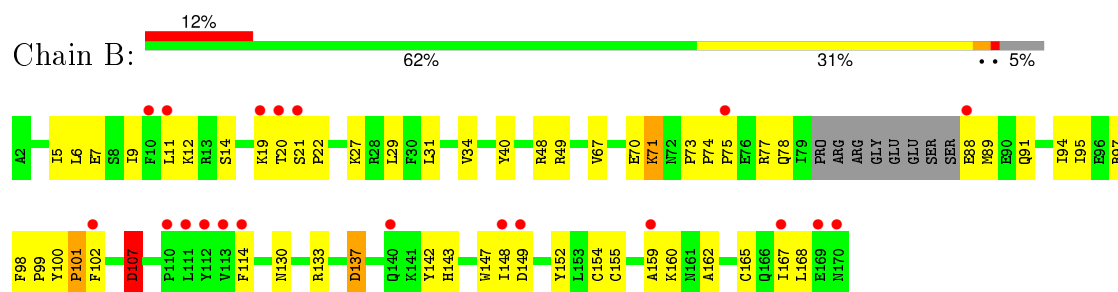e outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
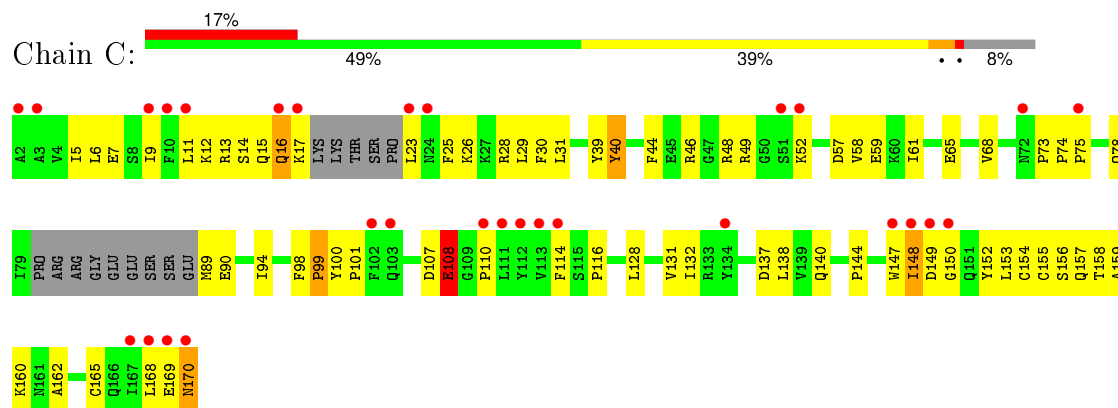
- Molecule 1: Tyrosine-protein kinase BTK

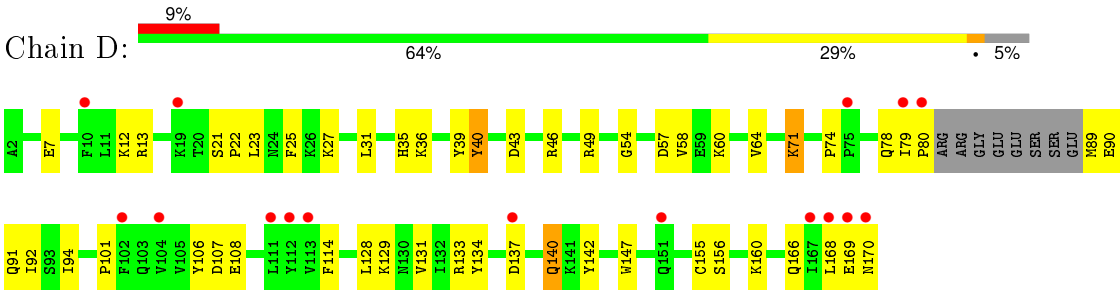- Molecule 1: Tyrosine-protein kinase BTK

- Molecule 1: Tyrosine-protein kinase BTK

- Molecule 1: Tyrosine-protein kinase BTK

Chain D:

64% 29% 5%

9%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.42Å 62.50Å 117.06Å 90.00° 94.33° 90.00°	Depositor
Resolution (Å)	29.67 – 2.58 29.67 – 2.58	Depositor EDS
% Data completeness (in resolution range)	98.1 (29.67-2.58) 98.2 (29.67-2.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$<I/\sigma(I)>$ [1]	7.84 (at 2.57Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.242 , 0.300 0.245 , 0.298	Depositor DCC
R_{free} test set	1283 reflections (5.07%)	DCC
Wilson B-factor (Å^2)	44.1	Xtriage
Anisotropy	0.764	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 58.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Outliers	0 of 26609 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5510	wwPDB-VP
Average B, all atoms (Å^2)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 33.69 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.6864e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, 4PT

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	0.41	0/1348	0.65	0/1817
1	B	0.41	0/1375	0.68	0/1852
1	C	0.36	0/1326	0.62	0/1785
1	D	0.43	0/1374	0.67	0/1852
All	All	0.40	0/5423	0.66	0/7306

There are no bond length outliers.

There are no bond angle outliers.

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	1316	0	1333	78	0
1	B	1343	0	1352	51	0
1	C	1296	0	1299	66	0
1	D	1341	0	1352	54	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	28	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	43	0	27	4	0
3	C	28	0	8	1	0
3	D	43	0	27	4	0
4	A	13	0	0	0	0
4	B	25	0	0	3	0
4	C	6	0	0	0	0
4	D	24	0	0	1	0
All	All	5510	0	5406	242	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 22.

All (242) 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:58:VAL:HG11	1:A:131:VAL:HG12	1.29	1.12
1:B:71:LYS:H	1:B:71:LYS:HE3	0.99	1.10
1:C:159:ALA:HB3	1:C:162:ALA:HB2	1.33	1.10
1:B:159:ALA:HB3	1:B:162:ALA:HB2	1.34	1.05
1:B:71:LYS:N	1:B:71:LYS:HE3	1.71	1.05
1:A:97:ARG:HH11	1:A:97:ARG:HB2	1.20	1.04
1:D:71:LYS:H	1:D:71:LYS:HE3	1.22	1.00
1:C:148:ILE:HD12	1:C:153:LEU:HD21	1.48	0.96
1:A:19:LYS:H	1:A:19:LYS:HD2	1.30	0.96
1:D:58:VAL:HG11	1:D:131:VAL:HG12	1.53	0.90
1:A:58:VAL:HG11	1:A:131:VAL:CG1	2.01	0.89
1:C:58:VAL:HG11	1:C:131:VAL:HG12	1.52	0.89
1:D:140:GLN:CD	1:D:140:GLN:H	1.78	0.87
1:A:26:LYS:HD3	1:A:28:ARG:HH22	1.42	0.83
1:D:71:LYS:H	1:D:71:LYS:CE	1.92	0.81
1:B:130:ASN:O	1:B:133:ARG:HG2	1.85	0.77
1:A:19:LYS:H	1:A:19:LYS:CD	1.94	0.76
1:D:58:VAL:HG11	1:D:131:VAL:CG1	2.16	0.75
1:C:152:TYR:HB3	1:C:154:CYS:SG	2.25	0.75
1:B:29:LEU:HD23	1:B:49:ARG:HG3	1.67	0.75
1:A:74:PRO:O	1:A:78:GLN:HG3	1.88	0.72
1:D:71:LYS:N	1:D:71:LYS:HE3	2.01	0.72
1:C:40:TYR:CE2	1:C:52:LYS:HG2	2.23	0.72
3:D:504:4PT:H0N2	3:D:504:4PT:H0C	1.72	0.71
1:C:17:LYS:HE2	1:C:108:GLU:HG2	1.72	0.71
1:C:89:MET:HG2	1:C:90:GLU:H	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ARG:HB2	1:A:97:ARG:NH1	2.00	0.70
1:C:58:VAL:CG1	1:C:131:VAL:HG12	2.22	0.69
1:B:74:PRO:O	1:B:78:GLN:HG3	1.93	0.69
3:D:504:4PT:O0H	3:D:504:4PT:H0E1	1.92	0.68
1:A:58:VAL:CG1	1:A:131:VAL:HG12	2.17	0.68
1:C:11:LEU:HB3	1:C:114:PHE:HB2	1.76	0.67
1:D:36:LYS:HA	1:D:58:VAL:HG23	1.76	0.66
1:C:12:LYS:HE2	3:C:503:4PT:O10	1.95	0.66
1:C:148:ILE:CD1	1:C:153:LEU:HD21	2.25	0.66
1:A:26:LYS:HB3	1:A:28:ARG:NH1	2.10	0.66
1:D:43:ASP:OD2	1:D:46:ARG:HB2	1.95	0.66
1:C:58:VAL:HG11	1:C:131:VAL:CG1	2.24	0.65
1:C:89:MET:HG2	1:C:90:GLU:N	2.11	0.64
1:B:7:GLU:HG3	1:B:31:LEU:CD2	2.27	0.64
1:B:75:PRO:N	1:B:78:GLN:HE21	1.96	0.64
3:B:502:4PT:O12	3:B:502:4PT:OP5	2.16	0.63
1:A:92:ILE:HD11	1:B:9:ILE:HG13	1.80	0.63
1:C:101:PRO:HB3	1:C:114:PHE:CD2	2.32	0.63
1:B:88:GLU:HB3	4:B:520:HOH:O	1.99	0.63
1:A:26:LYS:HD3	1:A:28:ARG:NH2	2.14	0.62
1:B:97:ARG:HD2	4:B:512:HOH:O	1.97	0.62
1:B:12:LYS:HE2	3:B:502:4PT:O10	1.99	0.62
1:C:99:PRO:O	1:C:101:PRO:HD3	2.00	0.62
1:D:7:GLU:HG3	1:D:31:LEU:CD2	2.29	0.62
1:A:26:LYS:HB3	1:A:28:ARG:HH12	1.64	0.61
1:C:101:PRO:HB3	1:C:114:PHE:CE2	2.36	0.61
1:B:11:LEU:HB3	1:B:114:PHE:HB2	1.82	0.61
1:A:101:PRO:HB3	1:A:114:PHE:CE2	2.35	0.61
1:B:11:LEU:HD23	1:B:77:ARG:HD3	1.84	0.60
1:B:147:TRP:CE3	1:B:160:LYS:HE3	2.37	0.59
1:A:19:LYS:N	1:A:19:LYS:HD2	2.08	0.59
1:A:97:ARG:HH11	1:A:97:ARG:CB	2.07	0.58
1:B:70:GLU:HB2	1:B:73:PRO:HG3	1.86	0.58
1:A:140:GLN:O	1:A:168:LEU:HB2	2.04	0.58
1:D:79:ILE:HB	1:D:80:PRO:HD3	1.83	0.58
1:C:5:ILE:HG22	1:C:6:LEU:HG	1.85	0.57
1:C:15:GLN:O	1:C:16:GLN:HB2	2.04	0.57
1:A:46:ARG:HD3	1:A:48:ARG:NH2	2.18	0.57
1:B:130:ASN:HA	1:B:133:ARG:HE	1.69	0.57
1:A:142:TYR:CD1	1:A:168:LEU:HD22	2.39	0.57
1:C:57:ASP:HB3	1:C:59:GLU:HG2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:ILE:HD11	1:C:153:LEU:HD11	1.86	0.57
1:A:43:ASP:OD2	1:A:46:ARG:HD2	2.04	0.56
1:B:148:ILE:HG22	1:B:149:ASP:OD2	2.05	0.56
1:A:97:ARG:HG2	1:A:99:PRO:HD3	1.86	0.56
1:A:147:TRP:HB2	1:A:152:TYR:CE1	2.39	0.56
1:D:140:GLN:CD	1:D:140:GLN:N	2.56	0.56
1:A:34:VAL:HB	1:D:134:TYR:CD2	2.40	0.56
1:C:17:LYS:HE2	1:C:108:GLU:CG	2.35	0.55
1:B:74:PRO:C	1:B:78:GLN:HE21	2.10	0.55
1:B:154:CYS:HB2	1:B:165:CYS:SG	2.46	0.55
1:A:148:ILE:O	1:A:149:ASP:HB2	2.07	0.55
1:A:89:MET:CE	1:A:90:GLU:H	2.21	0.54
1:C:94:ILE:HG23	1:D:91:GLN:HG3	1.88	0.54
1:A:64:VAL:O	1:A:65:GLU:HG2	2.07	0.54
1:C:74:PRO:C	1:C:78:GLN:HE21	2.11	0.54
1:A:140:GLN:CD	1:A:140:GLN:H	2.10	0.54
1:C:155:CYS:SG	1:C:157:GLN:HG3	2.48	0.54
1:B:71:LYS:C	1:B:73:PRO:HD3	2.28	0.54
1:A:75:PRO:N	1:A:78:GLN:HE21	2.05	0.53
1:D:142:TYR:CE1	1:D:168:LEU:HD23	2.43	0.53
1:C:58:VAL:HA	1:C:61:ILE:HD12	1.90	0.53
1:C:40:TYR:CD2	1:C:49:ARG:HD3	2.43	0.53
1:C:73:PRO:HG2	1:C:78:GLN:HG2	1.89	0.53
1:A:60:LYS:HE3	1:A:107:ASP:OD1	2.07	0.53
1:A:147:TRP:O	1:A:147:TRP:CE3	2.61	0.53
1:A:92:ILE:O	1:A:96:GLU:HG3	2.08	0.52
1:D:107:ASP:OD2	1:D:108:GLU:HG3	2.09	0.52
1:A:40:TYR:CD1	1:A:40:TYR:N	2.77	0.52
1:A:101:PRO:HB3	1:A:114:PHE:CD2	2.44	0.52
1:A:107:ASP:OD2	1:A:108:GLU:HG3	2.09	0.52
1:A:148:ILE:HG12	1:A:149:ASP:OD1	2.09	0.52
1:B:155:CYS:HB3	1:B:165:CYS:CB	2.40	0.52
1:B:5:ILE:HG22	1:B:6:LEU:HG	1.91	0.52
1:D:40:TYR:CD2	1:D:49:ARG:HD2	2.46	0.51
1:D:89:MET:CE	1:D:90:GLU:HB2	2.39	0.51
1:C:9:ILE:HG13	1:D:92:ILE:HD11	1.90	0.51
1:A:145:CYS:HB2	1:A:154:CYS:HB3	1.93	0.51
1:C:128:LEU:O	1:C:132:ILE:HG12	2.10	0.51
1:C:30:PHE:O	1:C:31:LEU:HD23	2.11	0.51
1:B:99:PRO:HG2	1:B:100:TYR:CE2	2.46	0.51
1:D:71:LYS:HE2	4:D:508:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:502:4PT:H0E2	3:B:502:4PT:H0P2	1.93	0.51
1:A:29:LEU:HD23	1:A:49:ARG:HB3	1.93	0.50
1:A:46:ARG:HD3	1:A:48:ARG:CZ	2.41	0.50
1:C:68:VAL:HG23	1:C:144:PRO:O	2.12	0.50
1:D:89:MET:HG3	1:D:90:GLU:N	2.27	0.50
1:C:44:PHE:O	1:D:27:LYS:HE3	2.12	0.50
1:C:147:TRP:NE1	1:C:160:LYS:HA	2.27	0.49
1:C:25:PHE:O	1:C:26:LYS:HG2	2.13	0.49
1:A:39:TYR:CZ	1:A:54:GLY:HA3	2.47	0.49
1:C:40:TYR:N	1:C:40:TYR:CD1	2.81	0.49
1:D:40:TYR:N	1:D:40:TYR:CD1	2.80	0.49
1:A:94:ILE:HD13	1:B:91:GLN:HB2	1.94	0.49
1:C:9:ILE:HG13	1:D:92:ILE:CD1	2.43	0.48
1:B:101:PRO:HB3	1:B:114:PHE:CD2	2.48	0.48
1:A:89:MET:HE2	1:A:90:GLU:H	1.77	0.48
1:C:7:GLU:HG3	1:C:31:LEU:CD2	2.43	0.48
1:D:12:LYS:HE3	1:D:39:TYR:CE2	2.48	0.48
1:B:7:GLU:HG3	1:B:31:LEU:HD23	1.94	0.48
1:A:59:GLU:HA	1:A:135:ASN:OD1	2.13	0.48
3:D:504:4PT:C0C	3:D:504:4PT:H0N2	2.35	0.48
1:A:14:SER:OG	3:A:501:4PT:H4	2.14	0.47
1:B:167:ILE:HG12	1:B:168:LEU:N	2.29	0.47
1:B:107:ASP:N	1:B:107:ASP:OD2	2.47	0.47
1:D:107:ASP:OD2	1:D:108:GLU:N	2.48	0.47
1:D:101:PRO:HB3	1:D:114:PHE:CE2	2.49	0.47
1:C:169:GLU:O	1:C:170:ASN:HB2	2.14	0.47
1:C:152:TYR:O	1:C:156:SER:N	2.38	0.47
1:A:8:SER:O	1:A:29:LEU:HD12	2.15	0.47
1:B:71:LYS:O	1:B:73:PRO:HD3	2.14	0.47
1:D:129:LYS:O	1:D:133:ARG:HG3	2.15	0.47
1:A:35:HIS:HA	1:D:35:HIS:HE1	1.79	0.47
1:A:67:VAL:HG12	1:A:102:PHE:HA	1.96	0.47
1:C:15:GLN:O	1:C:16:GLN:CB	2.63	0.46
1:B:137:ASP:N	1:B:137:ASP:OD1	2.47	0.46
1:B:34:VAL:HG22	4:B:508:HOH:O	2.15	0.46
1:B:101:PRO:HB3	1:B:114:PHE:CE2	2.51	0.46
1:C:170:ASN:C	1:C:170:ASN:HD22	2.18	0.46
1:A:25:PHE:N	1:A:25:PHE:CD1	2.83	0.46
1:D:89:MET:CG	1:D:90:GLU:H	2.28	0.46
1:A:71:LYS:C	1:A:73:PRO:HD3	2.36	0.46
1:C:29:LEU:O	1:C:39:TYR:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:VAL:CG1	1:D:131:VAL:HG12	2.33	0.46
1:C:74:PRO:O	1:C:78:GLN:HG3	2.16	0.46
1:D:89:MET:HE3	1:D:90:GLU:HB2	1.98	0.46
1:A:7:GLU:HG3	1:A:31:LEU:CD2	2.47	0.45
1:C:12:LYS:HG2	1:C:13:ARG:O	2.16	0.45
1:C:75:PRO:N	1:C:78:GLN:HE21	2.13	0.45
1:A:63:CYS:HB2	1:A:139:VAL:CG2	2.46	0.45
1:C:13:ARG:HG2	1:C:14:SER:N	2.32	0.45
1:A:75:PRO:HA	1:A:78:GLN:NE2	2.31	0.45
1:A:145:CYS:SG	1:A:154:CYS:HB3	2.57	0.45
1:C:99:PRO:HG2	1:C:100:TYR:CE2	2.51	0.45
1:C:5:ILE:O	1:C:6:LEU:HD23	2.16	0.45
1:D:169:GLU:OE2	1:D:169:GLU:HA	2.16	0.45
1:A:155:CYS:O	1:A:156:SER:HB2	2.17	0.45
1:A:52:LYS:HE3	1:A:55:SER:HB2	1.97	0.45
1:A:74:PRO:C	1:A:78:GLN:HE21	2.20	0.45
1:A:147:TRP:CZ3	1:A:160:LYS:NZ	2.85	0.45
1:A:147:TRP:O	1:A:147:TRP:HE3	2.00	0.45
1:D:89:MET:HG3	1:D:90:GLU:H	1.81	0.45
1:D:74:PRO:O	1:D:78:GLN:HG3	2.16	0.44
1:D:13:ARG:HD2	1:D:23:LEU:HD11	1.99	0.44
1:A:142:TYR:O	1:A:144:PRO:HD3	2.16	0.44
1:C:7:GLU:CG	1:C:29:LEU:HD11	2.47	0.44
1:D:21:SER:HA	1:D:22:PRO:HD3	1.76	0.44
1:C:154:CYS:HB2	1:C:165:CYS:SG	2.57	0.44
1:C:46:ARG:HD2	1:C:48:ARG:NH2	2.32	0.44
1:B:75:PRO:N	1:B:78:GLN:NE2	2.65	0.44
1:A:128:LEU:O	1:A:132:ILE:HG12	2.17	0.44
1:D:25:PHE:CD1	1:D:25:PHE:N	2.85	0.44
1:B:48:ARG:HB3	1:B:48:ARG:NH1	2.32	0.44
1:A:135:ASN:HB2	1:A:138:LEU:HD21	2.00	0.44
1:A:7:GLU:HG3	1:A:31:LEU:HD23	1.99	0.44
1:A:99:PRO:HG2	1:A:100:TYR:CE2	2.53	0.44
1:C:58:VAL:HG13	1:C:132:ILE:HG22	2.00	0.44
1:C:65:GLU:CD	1:C:168:LEU:HD11	2.38	0.44
1:B:99:PRO:O	1:B:101:PRO:HD3	2.18	0.43
1:D:7:GLU:HG3	1:D:31:LEU:HD23	2.00	0.43
1:B:147:TRP:HB2	1:B:152:TYR:CE1	2.53	0.43
1:A:72:ASN:N	1:A:73:PRO:HD3	2.33	0.43
1:D:169:GLU:O	1:D:170:ASN:HB2	2.17	0.43
1:C:155:CYS:O	1:C:156:SER:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:HB3	1:A:114:PHE:HB2	2.00	0.43
3:D:504:4PT:O0H	3:D:504:4PT:OP1	2.36	0.43
1:D:91:GLN:O	1:D:94:ILE:HG22	2.19	0.43
1:A:123:ARG:HH12	1:B:89:MET:CE	2.32	0.43
1:B:143:HIS:CD2	1:B:152:TYR:CE2	3.07	0.43
1:A:35:HIS:CE1	1:D:35:HIS:HA	2.53	0.43
1:B:31:LEU:HD11	1:B:49:ARG:HH11	1.84	0.43
1:C:26:LYS:HG3	1:C:28:ARG:HH21	1.84	0.43
1:D:39:TYR:CZ	1:D:54:GLY:HA3	2.54	0.42
1:B:21:SER:HA	1:B:22:PRO:HD3	1.85	0.42
1:A:35:HIS:HE1	1:D:35:HIS:HA	1.85	0.42
1:C:46:ARG:HD2	1:C:48:ARG:HH21	1.85	0.42
1:C:11:LEU:HB2	1:C:98:PHE:CG	2.54	0.42
1:A:92:ILE:CD1	1:B:9:ILE:HG13	2.49	0.42
1:A:142:TYR:CZ	1:A:144:PRO:HG3	2.55	0.42
1:C:116:PRO:HG3	1:D:91:GLN:NE2	2.34	0.42
1:D:106:TYR:CE2	1:D:108:GLU:HB2	2.54	0.42
1:B:155:CYS:HB3	1:B:165:CYS:HB3	2.01	0.42
1:B:40:TYR:CD1	1:B:40:TYR:N	2.86	0.42
1:C:13:ARG:HG2	1:C:14:SER:H	1.82	0.42
1:B:67:VAL:HG23	1:B:102:PHE:HA	2.02	0.42
1:C:17:LYS:HG2	1:C:108:GLU:HG2	2.01	0.42
1:A:21:SER:HA	1:A:22:PRO:HD3	1.73	0.42
1:A:68:VAL:HA	1:A:69:PRO:HD3	1.82	0.42
3:B:502:4PT:C0P	3:B:502:4PT:H0E2	2.45	0.41
1:D:89:MET:HE2	1:D:90:GLU:HB2	2.02	0.41
1:C:23:LEU:HD23	1:C:23:LEU:N	2.35	0.41
1:A:52:LYS:CE	1:A:55:SER:HB2	2.50	0.41
1:B:143:HIS:HB3	1:B:154:CYS:SG	2.60	0.41
1:B:152:TYR:HB3	1:B:154:CYS:SG	2.60	0.41
1:C:110:PRO:HD3	1:C:160:LYS:HG2	2.01	0.41
1:A:7:GLU:HA	1:A:30:PHE:O	2.19	0.41
1:C:23:LEU:O	1:C:23:LEU:HG	2.19	0.41
1:C:148:ILE:HG22	1:C:149:ASP:N	2.34	0.41
1:C:138:LEU:O	1:C:140:GLN:NE2	2.54	0.41
1:D:79:ILE:HG13	1:D:79:ILE:H	1.56	0.41
1:A:35:HIS:HA	1:D:35:HIS:CE1	2.55	0.41
1:D:57:ASP:HB2	1:D:60:LYS:HG3	2.03	0.41
1:A:68:VAL:O	1:A:146:PHE:CE2	2.74	0.41
1:B:94:ILE:HG23	1:B:95:ILE:HG23	2.02	0.41
1:B:27:LYS:HE2	1:B:98:PHE:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:ASN:HA	1:B:133:ARG:NE	2.36	0.41
1:A:40:TYR:CD2	1:A:52:LYS:HA	2.56	0.41
1:C:7:GLU:HA	1:C:30:PHE:O	2.20	0.41
1:D:23:LEU:HD22	1:D:23:LEU:HA	1.90	0.41
1:D:147:TRP:CZ3	1:D:160:LYS:NZ	2.87	0.41
1:D:36:LYS:CA	1:D:58:VAL:HG23	2.48	0.41
1:A:63:CYS:HB2	1:A:139:VAL:HG22	2.02	0.41
1:D:64:VAL:HG21	1:D:128:LEU:HB3	2.03	0.41
1:B:147:TRP:CD2	1:B:160:LYS:HE3	2.56	0.40
1:A:64:VAL:HG21	1:A:128:LEU:HB3	2.03	0.40
1:D:155:CYS:O	1:D:156:SER:HB2	2.22	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	154/169 (91%)	139 (90%)	15 (10%)	0	100	100
1	B	157/169 (93%)	141 (90%)	14 (9%)	2 (1%)	15	29
1	C	149/169 (88%)	130 (87%)	13 (9%)	6 (4%)	4	4
1	D	157/169 (93%)	147 (94%)	10 (6%)	0	100	100
All	All	617/676 (91%)	557 (90%)	52 (8%)	8 (1%)	15	29

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	19	LYS
1	C	16	GLN
1	C	107	ASP
1	C	108	GLU

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Mol	Chain	Res	Type
1	C	150	GLY
1	B	107	ASP
1	C	148	ILE
1	C	99	PRO

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	148/158 (94%)	140 (95%)	8 (5%)	27	51
1	B	151/158 (96%)	144 (95%)	7 (5%)	33	59
1	C	145/158 (92%)	140 (97%)	5 (3%)	44	71
1	D	151/158 (96%)	146 (97%)	5 (3%)	45	71
All	All	595/632 (94%)	570 (96%)	25 (4%)	36	63

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LYS
1	A	40	TYR
1	A	67	VAL
1	A	70	GLU
1	A	97	ARG
1	A	140	GLN
1	A	151	GLN
1	A	168	LEU
1	B	14	SER
1	B	20	THR
1	B	71	LYS
1	B	101	PRO
1	B	107	ASP
1	B	137	ASP
1	B	142	TYR
1	C	40	TYR
1	C	108	GLU

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Mol	Chain	Res	Type
1	C	137	ASP
1	C	158	THR
1	C	170	ASN
1	D	40	TYR
1	D	71	LYS
1	D	137	ASP
1	D	140	GLN
1	D	166	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	151	GLN
1	B	78	GLN
1	C	78	GLN
1	C	140	GLN
1	D	78	GLN
1	D	127	GLN
1	D	130	ASN
1	D	151	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)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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	4PT	A	501	-	28,28,43	1.46	3 (10%)	38,46,64	0.80	1 (2%)
3	4PT	B	502	-	43,43,43	1.50	4 (9%)	52,64,64	1.32	5 (9%)
3	4PT	C	503	-	28,28,43	1.45	3 (10%)	38,46,64	0.81	1 (2%)
3	4PT	D	504	-	43,43,43	1.49	4 (9%)	52,64,64	1.22	3 (5%)

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	4PT	A	501	-	-	0/20/44/65	0/1/1/1
3	4PT	B	502	-	2/2/13/13	0/40/65/65	0/1/1/1
3	4PT	C	503	-	-	0/20/44/65	0/1/1/1
3	4PT	D	504	-	2/2/13/13	0/40/65/65	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	4PT	C0I-C0G	-5.25	1.39	1.50
3	D	504	4PT	C0I-C0G	-5.24	1.39	1.50
3	D	504	4PT	P3-O12	3.09	1.61	1.51
3	D	504	4PT	P5-OP9	3.10	1.61	1.51
3	B	502	4PT	P3-O12	3.10	1.61	1.51
3	B	502	4PT	P5-OP9	3.11	1.61	1.51
3	A	501	4PT	P5-OP9	3.12	1.61	1.51
3	C	503	4PT	P5-OP9	3.13	1.61	1.51
3	B	502	4PT	P4-OP4	3.13	1.61	1.51
3	A	501	4PT	P3-O12	3.14	1.61	1.51
3	D	504	4PT	P4-OP4	3.14	1.61	1.51
3	C	503	4PT	P3-O12	3.14	1.61	1.51
3	C	503	4PT	P1-OP2	3.15	1.61	1.51
3	A	501	4PT	P1-OP2	3.16	1.61	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	502	4PT	C0B-C0C-C0E	-2.94	105.19	112.07
3	B	502	4PT	C0E-O0F-C0L	-2.48	109.92	116.85
3	A	501	4PT	O4-P4-OP4	2.32	112.91	107.11
3	C	503	4PT	O4-P4-OP4	2.52	113.41	107.11
3	B	502	4PT	O0F-C0L-C0N	2.81	120.45	111.90
3	B	502	4PT	C0J-C0I-C0G	2.84	119.17	113.87
3	D	504	4PT	O0F-C0L-C0N	2.98	120.97	111.90
3	D	504	4PT	C0J-C0I-C0G	3.14	119.73	113.87
3	B	502	4PT	O0H-C0G-C0I	5.43	118.85	109.05
3	D	504	4PT	O0H-C0G-C0I	5.70	119.33	109.05

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	502	4PT	C0G
3	B	502	4PT	C0C
3	D	504	4PT	C0G
3	D	504	4PT	C0C

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	4PT	1	0
3	B	502	4PT	4	0
3	C	503	4PT	1	0
3	D	504	4PT	4	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	158/169 (93%)	0.80	25 (15%)	3	2	31, 50, 81, 88	0
1	B	161/169 (95%)	0.66	20 (12%)	5	4	24, 47, 77, 91	0
1	C	155/169 (91%)	1.04	29 (18%)	2	1	36, 59, 85, 99	0
1	D	161/169 (95%)	0.49	16 (9%)	9	7	23, 44, 65, 92	0
All	All	635/676 (93%)	0.75	90 (14%)	4	2	23, 50, 80, 99	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	19	LYS	7.2
1	C	170	ASN	5.8
1	C	149	ASP	5.0
1	C	113	VAL	4.6
1	C	148	ILE	4.4
1	A	20	THR	4.4
1	B	88	GLU	4.2
1	A	149	ASP	4.2
1	C	102	PHE	4.0
1	A	113	VAL	3.9
1	D	170	ASN	3.9
1	A	72	ASN	3.7
1	A	104	VAL	3.7
1	D	169	GLU	3.5
1	D	80	PRO	3.5
1	C	3	ALA	3.4
1	C	51	SER	3.3
1	C	134	TYR	3.3
1	D	111	LEU	3.3
1	C	147	TRP	3.2
1	A	51	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	102	PHE	3.1
1	C	114	PHE	3.1
1	A	150	GLY	3.1
1	D	168	LEU	3.1
1	A	75	PRO	3.0
1	C	167	ILE	3.0
1	B	75	PRO	3.0
1	B	167	ILE	3.0
1	C	2	ALA	3.0
1	D	104	VAL	3.0
1	C	10	PHE	3.0
1	C	17	LYS	3.0
1	A	168	LEU	2.9
1	D	113	VAL	2.8
1	C	16	GLN	2.8
1	A	10	PHE	2.8
1	C	112	TYR	2.7
1	D	79	ILE	2.7
1	C	11	LEU	2.7
1	B	113	VAL	2.7
1	B	170	ASN	2.7
1	A	119	GLU	2.6
1	B	111	LEU	2.6
1	C	110	PRO	2.6
1	A	17	LYS	2.5
1	D	167	ILE	2.5
1	C	111	LEU	2.5
1	B	112	TYR	2.5
1	B	159	ALA	2.4
1	A	158	THR	2.4
1	B	169	GLU	2.4
1	C	169	GLU	2.4
1	D	112	TYR	2.4
1	C	9	ILE	2.4
1	A	11	LEU	2.4
1	C	52	LYS	2.4
1	C	103	GLN	2.4
1	C	150	GLY	2.3
1	D	19	LYS	2.3
1	D	75	PRO	2.3
1	C	23	LEU	2.3
1	C	72	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	148	ILE	2.2
1	A	21	SER	2.2
1	B	11	LEU	2.2
1	B	114	PHE	2.2
1	B	21	SER	2.2
1	B	102	PHE	2.2
1	D	10	PHE	2.2
1	A	46	ARG	2.2
1	B	110	PRO	2.2
1	B	20	THR	2.2
1	B	10	PHE	2.1
1	B	140	GLN	2.1
1	A	89	MET	2.1
1	A	114	PHE	2.1
1	B	149	ASP	2.1
1	A	19	LYS	2.1
1	A	151	GLN	2.1
1	D	137	ASP	2.1
1	C	168	LEU	2.1
1	C	24	ASN	2.1
1	A	153	LEU	2.1
1	A	16	GLN	2.0
1	A	112	TYR	2.0
1	A	140	GLN	2.0
1	C	75	PRO	2.0
1	D	151	GLN	2.0
1	D	102	PHE	2.0

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

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

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.

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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
3	4PT	D	504	43/43	0.95	0.18	0.11	33,47,84,86	0
3	4PT	B	502	43/43	0.93	0.20	-0.15	42,62,76,77	0
3	4PT	A	501	28/43	0.92	0.19	-0.62	60,71,77,79	0
3	4PT	C	503	28/43	0.88	0.22	-0.83	103,108,110,111	0
2	ZN	C	303	1/1	0.96	0.08	-2.47	55,55,55,55	0
2	ZN	D	304	1/1	0.99	0.07	-2.63	36,36,36,36	0
2	ZN	A	301	1/1	0.98	0.06	-3.02	44,44,44,44	0
2	ZN	B	302	1/1	0.98	0.05	-3.10	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.