Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 10:21 AM EDT

PDB ID	:	2IBG
Title	:	Crystal Structure of Hedgehog Bound to the FNIII Domains of Ihog
Authors	:	McLellan, J.S.; Leahy, D.J.
Deposited on	:	2006-09-11
Resolution	:	2.20 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 (1)) were used in the production of this report:

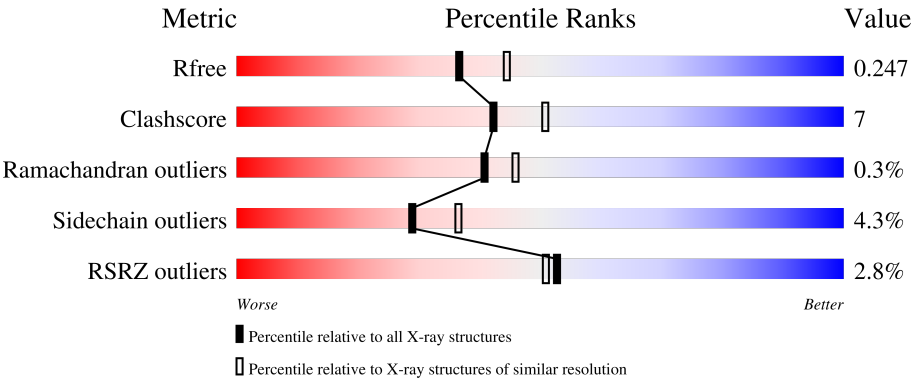
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	214	86% 13% •
1	B	214	% 83% 15%
1	C	214	% 87% 12%
1	D	214	90% 9%
2	E	150	% 76% 17% • 5%

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Mol	Chain	Length	Quality of chain
2	F	150	12% 53% 27% 7% 12%
2	G	150	3% 63% 25% 11%
2	H	150	4% 73% 19% 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11644 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 CG9211-PA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	214	Total	C	N	O	S	0	0	0
			1715	1095	290	325	5			
1	B	213	Total	C	N	O	S	0	0	0
			1705	1089	288	323	5			
1	C	213	Total	C	N	O	S	0	0	0
			1705	1089	288	323	5			
1	D	213	Total	C	N	O	S	0	0	0
			1705	1089	288	323	5			

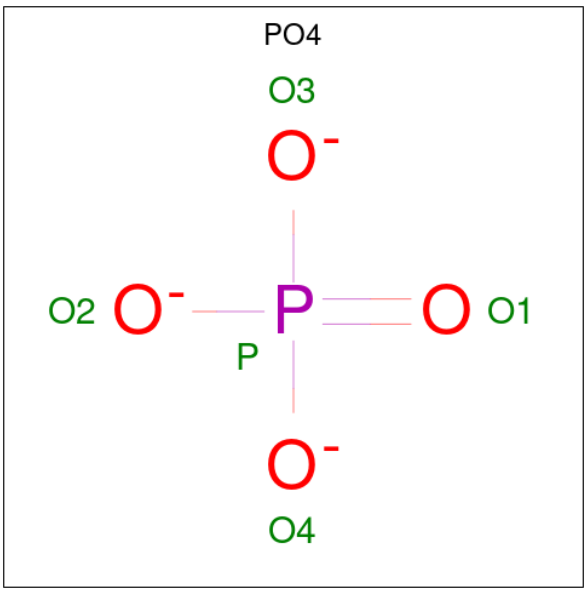
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	464	SER	-	cloning artifact	UNP Q9VM64
A	465	THR	-	cloning artifact	UNP Q9VM64
B	464	SER	-	cloning artifact	UNP Q9VM64
B	465	THR	-	cloning artifact	UNP Q9VM64
C	464	SER	-	cloning artifact	UNP Q9VM64
C	465	THR	-	cloning artifact	UNP Q9VM64
D	464	SER	-	cloning artifact	UNP Q9VM64
D	465	THR	-	cloning artifact	UNP Q9VM64

- Molecule 2 is a protein called Protein hedgehog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	142	Total	C	N	O	S	0	0	0
			1161	732	206	218	5			
2	F	132	Total	C	N	O	S	0	0	0
			1070	679	190	196	5			
2	G	134	Total	C	N	O	S	0	0	0
			1092	694	191	202	5			
2	H	140	Total	C	N	O	S	0	0	0
			1142	722	201	214	5			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 4 is water.

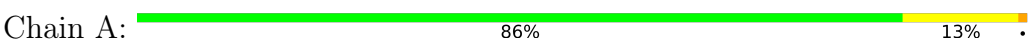
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	66	Total O 66 66	0	0
4	B	48	Total O 48 48	0	0
4	C	63	Total O 63 63	0	0
4	D	54	Total O 54 54	0	0
4	E	28	Total O 28 28	0	0
4	F	8	Total O 8 8	0	0
4	G	12	Total O 12 12	0	0
4	H	10	Total O 10 10	0	0

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.

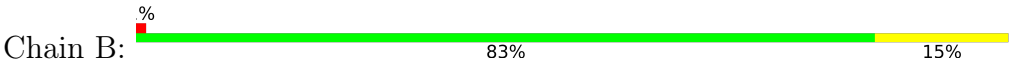
• Molecule 1: CG9211-PA

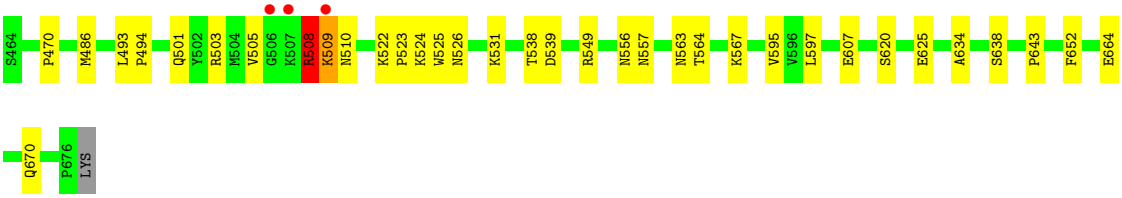
Chain A:



• Molecule 1: CG9211-PA

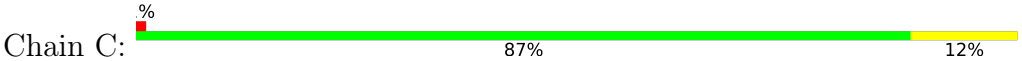
Chain B:

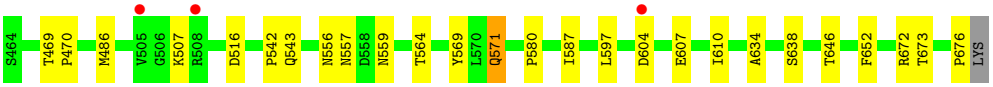




• Molecule 1: CG9211-PA

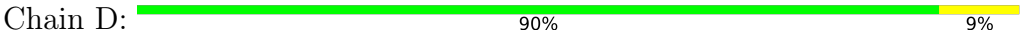
Chain C:





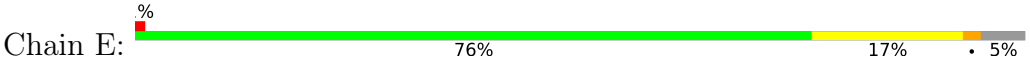
• Molecule 1: CG9211-PA

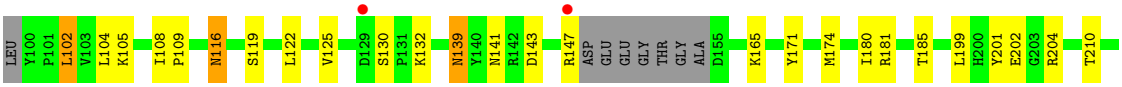
Chain D:



• Molecule 2: Protein hedgehog

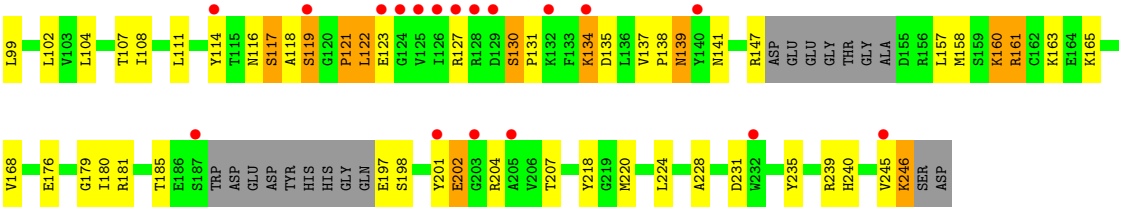
Chain E:





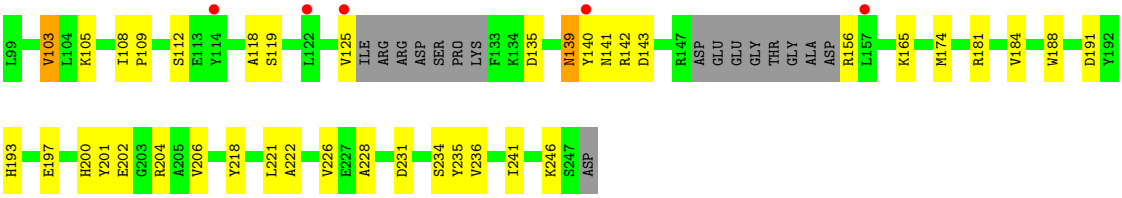
• Molecule 2: Protein hedgehog

Chain F:



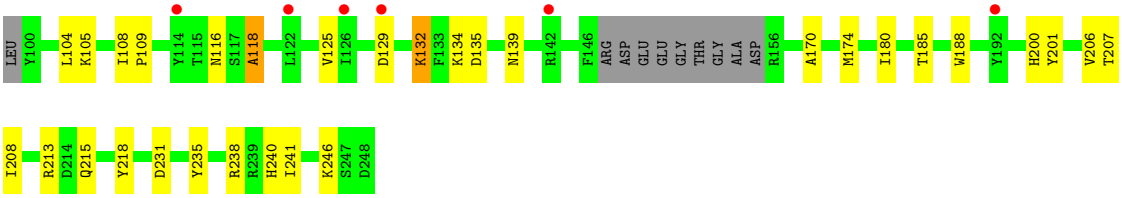
• Molecule 2: Protein hedgehog

Chain G:



• Molecule 2: Protein hedgehog

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.35Å 70.00Å 155.69Å 90.00° 90.18° 90.00°	Depositor
Resolution (Å)	37.68 – 2.20 37.68 – 2.20	Depositor EDS
% Data completeness (in resolution range)	92.2 (37.68-2.20) 92.1 (37.68-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.198 , 0.246 0.200 , 0.247	Depositor DCC
R_{free} test set	4169 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	30.4	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 42.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.074 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11644	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.49% 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: 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	0.68	0/1764	0.73	0/2397
1	B	0.64	0/1754	0.68	0/2386
1	C	0.60	0/1754	0.67	0/2386
1	D	0.64	0/1754	0.71	0/2386
2	E	0.51	0/1187	0.66	1/1603 (0.1%)
2	F	1.98	31/1090 (2.8%)	1.07	7/1470 (0.5%)
2	G	0.52	0/1116	0.60	0/1508
2	H	0.48	0/1168	0.61	0/1578
All	All	0.83	31/11587 (0.3%)	0.72	8/15714 (0.1%)

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
2	F	0	1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	117	SER	CB-OG	23.21	1.72	1.42
2	F	202	GLU	CD-OE2	20.15	1.47	1.25
2	F	161	ARG	CZ-NH1	18.89	1.57	1.33
2	F	123	GLU	CD-OE1	17.42	1.44	1.25
2	F	121	PRO	C-N	15.07	1.68	1.34
2	F	197	GLU	CD-OE1	10.91	1.37	1.25
2	F	197	GLU	CG-CD	10.39	1.67	1.51
2	F	161	ARG	NE-CZ	9.84	1.45	1.33
2	F	114	TYR	CG-CD2	9.60	1.51	1.39
2	F	197	GLU	CD-OE2	9.58	1.36	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	197	GLU	C-O	9.56	1.41	1.23
2	F	114	TYR	CE1-CZ	9.26	1.50	1.38
2	F	246	LYS	C-O	9.23	1.40	1.23
2	F	114	TYR	CE2-CZ	9.04	1.50	1.38
2	F	119	SER	CB-OG	8.99	1.53	1.42
2	F	117	SER	C-N	8.62	1.53	1.34
2	F	135	ASP	CG-OD1	8.37	1.44	1.25
2	F	114	TYR	CG-CD1	8.29	1.50	1.39
2	F	123	GLU	CD-OE2	7.29	1.33	1.25
2	F	130	SER	CA-CB	6.95	1.63	1.52
2	F	122	LEU	C-O	6.37	1.35	1.23
2	F	116	ASN	C-O	6.34	1.35	1.23
2	F	161	ARG	CG-CD	6.09	1.67	1.51
2	F	165	LYS	CD-CE	6.08	1.66	1.51
2	F	161	ARG	CZ-NH2	6.08	1.41	1.33
2	F	117	SER	C-O	5.57	1.33	1.23
2	F	134	LYS	CD-CE	5.42	1.64	1.51
2	F	130	SER	C-O	5.39	1.33	1.23
2	F	201	TYR	CG-CD1	5.36	1.46	1.39
2	F	131	PRO	N-CD	5.28	1.55	1.47
2	F	201	TYR	CE2-CZ	5.08	1.45	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	161	ARG	NE-CZ-NH2	-19.50	110.55	120.30
2	F	121	PRO	O-C-N	8.21	135.84	122.70
2	F	121	PRO	CA-C-N	-6.54	102.82	117.20
2	F	161	ARG	NE-CZ-NH1	5.83	123.21	120.30
2	F	161	ARG	NH1-CZ-NH2	5.30	125.23	119.40
2	F	122	LEU	CA-CB-CG	5.24	127.36	115.30
2	E	102	LEU	CA-CB-CG	5.19	127.23	115.30
2	F	202	GLU	OE1-CD-OE2	-5.10	117.18	123.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	202	GLU	Sidechain

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	1715	0	1674	25	0
1	B	1705	0	1661	21	0
1	C	1705	0	1661	15	0
1	D	1705	0	1661	18	0
2	E	1161	0	1137	16	0
2	F	1070	0	1080	29	0
2	G	1092	0	1073	22	0
2	H	1142	0	1120	18	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	5	0	0	0	0
3	E	15	0	0	0	0
3	F	5	0	0	1	0
3	H	5	0	0	0	0
4	A	66	0	0	2	0
4	B	48	0	0	0	0
4	C	63	0	0	1	0
4	D	54	0	0	1	0
4	E	28	0	0	0	0
4	F	8	0	0	0	0
4	G	12	0	0	0	0
4	H	10	0	0	0	0
All	All	11644	0	11067	154	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 7.

All (154) 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)
2:F:121:PRO:C	2:F:122:LEU:N	1.68	1.46
2:F:117:SER:CB	2:F:117:SER:OG	1.72	1.34
2:H:185:THR:OG1	2:H:207:THR:HG22	1.68	0.93
1:C:580:PRO:HG2	1:C:610:ILE:HD11	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:168:VAL:HG23	2:F:228:ALA:HB1	1.67	0.76
1:D:542:PRO:HB3	4:D:274:HOH:O	1.87	0.72
2:G:125:VAL:HG13	2:G:201:TYR:HB3	1.72	0.72
1:A:620:SER:HB3	1:A:670:GLN:NE2	2.05	0.72
2:E:147:ARG:HG2	2:E:185:THR:HA	1.72	0.70
2:F:121:PRO:CA	2:F:122:LEU:N	2.55	0.69
2:G:221:LEU:HD23	2:G:241:ILE:HD12	1.76	0.68
1:B:607:GLU:HG2	1:B:634:ALA:HB1	1.76	0.66
2:F:139:ASN:HD22	2:F:141:ASN:H	1.45	0.64
1:A:484:ARG:NH2	1:D:528:GLU:HB3	2.11	0.64
1:B:505:VAL:HG21	1:B:567:LYS:HG2	1.79	0.62
2:H:125:VAL:HG13	2:H:201:TYR:HB3	1.80	0.62
2:G:118:ALA:O	2:G:231:ASP:HB3	2.00	0.62
1:A:620:SER:HB3	1:A:670:GLN:HE22	1.63	0.61
1:A:489:ARG:CB	1:D:472:ASN:OD1	2.48	0.61
1:B:501:GLN:HE22	1:B:549:ARG:HH21	1.49	0.61
1:D:551:LEU:HD22	2:G:103:VAL:HG13	1.82	0.61
2:F:160:LYS:HA	2:F:160:LYS:HE3	1.83	0.60
2:G:234:SER:OG	2:G:236:VAL:HG22	2.02	0.60
2:E:125:VAL:HG13	2:E:201:TYR:HB3	1.84	0.60
1:D:489:ARG:NH1	1:D:528:GLU:O	2.35	0.59
2:E:139:ASN:ND2	2:E:141:ASN:H	2.01	0.59
2:F:185:THR:OG1	2:F:207:THR:HG22	2.03	0.59
1:C:607:GLU:HG2	1:C:634:ALA:HB1	1.84	0.58
1:A:620:SER:CB	1:A:670:GLN:NE2	2.65	0.58
2:E:139:ASN:HD21	2:E:141:ASN:HB2	1.68	0.58
2:F:119:SER:O	2:F:246:LYS:HA	2.03	0.58
2:E:122:LEU:HD23	2:E:199:LEU:HD23	1.86	0.58
2:F:121:PRO:C	2:F:122:LEU:CA	2.70	0.57
2:E:116:ASN:OD1	2:E:116:ASN:N	2.37	0.57
2:F:179:GLY:HA2	3:F:410:PO4:P	2.44	0.56
1:B:486:MET:SD	1:C:486:MET:SD	3.04	0.56
1:A:489:ARG:HB2	1:D:472:ASN:OD1	2.06	0.55
2:H:104:LEU:O	2:H:105:LYS:HB2	2.06	0.55
1:A:528:GLU:HG2	1:D:632:GLU:HG2	1.87	0.55
2:H:206:VAL:HG22	2:H:208:ILE:HG23	1.89	0.55
2:E:139:ASN:HD21	2:E:141:ASN:CB	2.19	0.55
1:C:516:ASP:O	4:C:239:HOH:O	2.19	0.54
2:E:104:LEU:HG	2:E:105:LYS:HG2	1.88	0.54
1:B:501:GLN:HE21	1:B:549:ARG:HE	1.55	0.54
1:A:489:ARG:HB3	1:D:472:ASN:OD1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:587:ILE:HD13	1:C:652:PHE:CD1	2.44	0.53
1:A:507:LYS:O	1:A:509:LYS:HG2	2.09	0.52
1:C:556:ASN:O	1:C:557:ASN:HB2	2.09	0.52
1:A:664:GLU:HG3	4:A:79:HOH:O	2.10	0.52
2:F:137:VAL:HG21	2:F:160:LYS:HZ1	1.75	0.52
2:G:191:ASP:HB3	2:G:193:HIS:CD2	2.45	0.52
1:A:607:GLU:HG2	1:A:634:ALA:HB1	1.93	0.51
2:E:139:ASN:C	2:E:139:ASN:HD22	2.15	0.51
2:F:204:ARG:HG2	2:F:245:VAL:HG23	1.91	0.51
1:A:556:ASN:O	1:A:557:ASN:HB2	2.11	0.50
1:B:522:LYS:HB3	1:B:523:PRO:HA	1.93	0.50
1:A:472:ASN:OD1	1:D:489:ARG:HB3	2.10	0.50
1:A:542:PRO:HB3	4:A:25:HOH:O	2.11	0.50
1:B:470:PRO:HG3	1:B:563:ASN:HB2	1.94	0.50
1:B:501:GLN:NE2	1:B:549:ARG:HE	2.09	0.50
1:D:580:PRO:HG2	1:D:610:ILE:HD11	1.93	0.50
1:B:503:ARG:HD3	1:B:509:LYS:HG3	1.94	0.50
1:D:489:ARG:NH1	1:D:528:GLU:C	2.66	0.49
2:E:143:ASP:HB3	2:E:174:MET:CE	2.43	0.49
1:A:470:PRO:HG3	1:A:563:ASN:HB2	1.95	0.49
1:B:503:ARG:CD	1:B:509:LYS:HG3	2.43	0.49
2:H:231:ASP:CG	2:H:246:LYS:HG3	2.32	0.48
1:B:597:LEU:O	1:B:638:SER:HA	2.13	0.48
2:G:119:SER:O	2:G:246:LYS:HA	2.13	0.48
2:H:118:ALA:O	2:H:231:ASP:HB3	2.14	0.48
2:F:158:MET:CE	2:F:163:LYS:HA	2.43	0.48
2:H:207:THR:HG23	2:H:240:HIS:CG	2.48	0.47
2:G:231:ASP:CG	2:G:246:LYS:HG3	2.34	0.47
1:B:508:ARG:O	1:B:510:ASN:N	2.48	0.47
1:B:524:LYS:HE3	1:B:525:TRP:CZ2	2.50	0.47
2:F:127:ARG:H	2:F:130:SER:HB2	1.80	0.47
1:C:580:PRO:CG	1:C:610:ILE:HD11	2.40	0.47
1:D:489:ARG:NH1	1:D:528:GLU:HA	2.30	0.47
1:D:592:GLU:O	1:D:646:THR:HA	2.15	0.47
1:C:672:ARG:HD2	1:C:673:THR:O	2.15	0.46
2:G:108:ILE:HA	2:G:109:PRO:C	2.35	0.46
2:H:170:ALA:O	2:H:174:MET:HG3	2.14	0.46
2:F:102:LEU:HD11	2:F:108:ILE:HD12	1.97	0.46
2:F:139:ASN:ND2	2:F:141:ASN:H	2.11	0.46
2:F:220:MET:O	2:F:220:MET:HE3	2.15	0.46
2:H:208:ILE:HG13	2:H:241:ILE:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:SER:OG	1:A:670:GLN:NE2	2.49	0.46
1:B:595:VAL:HG21	1:B:652:PHE:CZ	2.51	0.45
2:G:191:ASP:HB3	2:G:193:HIS:HD2	1.80	0.45
1:C:559:ASN:HD21	2:H:104:LEU:H	1.63	0.45
2:G:139:ASN:ND2	2:G:141:ASN:H	2.14	0.45
2:H:188:TRP:HA	2:H:200:HIS:O	2.17	0.45
2:G:202:GLU:HB2	2:G:204:ARG:HG3	1.98	0.45
2:F:207:THR:HG23	2:F:240:HIS:CD2	2.52	0.45
2:G:105:LYS:HA	2:G:105:LYS:HD3	1.82	0.45
1:B:556:ASN:O	1:B:557:ASN:HB2	2.16	0.45
2:G:143:ASP:CG	2:G:174:MET:HE1	2.37	0.45
1:C:646:THR:HG21	1:C:676:PRO:HG3	1.98	0.45
2:F:176:GLU:HG3	2:F:224:LEU:HD11	1.99	0.45
2:E:171:TYR:HA	2:E:174:MET:HE3	1.99	0.45
1:B:620:SER:OG	1:B:670:GLN:NE2	2.50	0.45
1:C:597:LEU:O	1:C:638:SER:HA	2.16	0.44
1:D:542:PRO:O	1:D:543:GLN:HB2	2.16	0.44
1:B:664:GLU:OE2	1:B:664:GLU:HA	2.18	0.44
1:A:504:MET:HB2	1:A:509:LYS:HG3	2.00	0.44
1:B:538:THR:O	1:B:539:ASP:HB2	2.17	0.44
2:E:139:ASN:HD22	2:E:141:ASN:H	1.65	0.44
2:F:218:TYR:HE2	2:F:239:ARG:O	2.00	0.44
1:A:620:SER:OG	1:A:649:MET:HG3	2.17	0.44
2:G:142:ARG:O	2:G:142:ARG:HG2	2.17	0.44
1:B:526:ASN:OD1	1:B:531:LYS:HA	2.18	0.44
2:E:143:ASP:O	2:E:181:ARG:HD2	2.17	0.44
1:C:507:LYS:H	1:C:507:LYS:HG2	1.70	0.43
2:F:147:ARG:HB3	2:F:185:THR:HA	2.00	0.43
2:F:158:MET:HE1	2:F:163:LYS:HA	2.00	0.43
2:G:165:LYS:HG3	2:G:228:ALA:O	2.18	0.43
2:F:180:ILE:HD12	2:F:180:ILE:N	2.33	0.43
2:H:108:ILE:HA	2:H:109:PRO:C	2.38	0.43
2:H:207:THR:HG23	2:H:240:HIS:HB2	2.00	0.43
1:C:569:TYR:CE2	1:C:571:GLN:NE2	2.86	0.43
1:B:523:PRO:HD3	1:B:643:PRO:HD2	1.99	0.43
2:F:118:ALA:O	2:F:231:ASP:HB3	2.18	0.43
2:G:184:VAL:HG13	2:G:206:VAL:HG23	1.99	0.43
2:H:215:GLN:NE2	2:H:238:ARG:O	2.52	0.43
1:C:542:PRO:C	1:C:543:GLN:HG2	2.39	0.42
1:D:541:LYS:HA	1:D:542:PRO:HD3	1.87	0.42
2:E:180:ILE:HD12	2:E:210:THR:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:161:ARG:HH21	2:F:231:ASP:CG	2.23	0.42
2:G:234:SER:OG	2:G:236:VAL:CG2	2.67	0.42
1:A:597:LEU:O	1:A:638:SER:HA	2.19	0.42
1:D:505:VAL:HG22	1:D:545:THR:HB	2.02	0.42
2:H:206:VAL:CG2	2:H:208:ILE:HG23	2.49	0.42
2:H:213:ARG:HA	2:H:218:TYR:OH	2.20	0.42
2:F:134:LYS:HD3	2:F:134:LYS:H	1.85	0.41
2:F:176:GLU:HG3	2:F:224:LEU:HD21	2.02	0.41
1:A:484:ARG:HD2	1:A:614:TYR:OH	2.20	0.41
2:G:139:ASN:HD22	2:G:140:TYR:N	2.18	0.41
1:D:597:LEU:O	1:D:638:SER:HA	2.20	0.41
2:G:188:TRP:HA	2:G:200:HIS:O	2.20	0.41
2:H:132:LYS:HE3	2:H:132:LYS:HA	2.03	0.41
1:A:509:LYS:HA	1:A:509:LYS:HD3	1.83	0.41
2:H:104:LEU:HG	2:H:105:LYS:HG2	2.03	0.41
1:A:465:THR:HB	1:A:554:TYR:CZ	2.56	0.41
1:A:504:MET:HE2	1:A:504:MET:HB3	1.94	0.41
2:G:218:TYR:HB3	2:G:241:ILE:HD11	2.03	0.41
2:G:222:ALA:O	2:G:226:VAL:HG23	2.21	0.41
1:A:559:ASN:HD21	2:F:104:LEU:H	1.69	0.40
1:D:518:ILE:HD12	1:D:518:ILE:H	1.86	0.40
2:E:108:ILE:HA	2:E:109:PRO:C	2.40	0.40
2:F:139:ASN:HA	2:F:163:LYS:HE3	2.03	0.40
2:E:202:GLU:HG3	2:E:204:ARG:HG3	2.03	0.40
1:A:552:ALA:O	1:A:559:ASN:HA	2.22	0.40
1:B:493:LEU:HA	1:B:494:PRO:HD3	1.94	0.40
1:C:469:THR:HB	1:C:470:PRO:HD2	2.04	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	212/214 (99%)	208 (98%)	4 (2%)	0	100	100
1	B	211/214 (99%)	207 (98%)	2 (1%)	2 (1%)	17	16
1	C	211/214 (99%)	206 (98%)	5 (2%)	0	100	100
1	D	211/214 (99%)	206 (98%)	5 (2%)	0	100	100
2	E	138/150 (92%)	136 (99%)	2 (1%)	0	100	100
2	F	126/150 (84%)	118 (94%)	7 (6%)	1 (1%)	19	19
2	G	128/150 (85%)	122 (95%)	6 (5%)	0	100	100
2	H	136/150 (91%)	128 (94%)	7 (5%)	1 (1%)	22	22
All	All	1373/1456 (94%)	1331 (97%)	38 (3%)	4 (0%)	41	46

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	509	LYS
1	B	508	ARG
2	F	198	SER
2	H	118	ALA

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	186/186 (100%)	177 (95%)	9 (5%)	25	32
1	B	185/186 (100%)	182 (98%)	3 (2%)	62	76
1	C	185/186 (100%)	182 (98%)	3 (2%)	62	76
1	D	185/186 (100%)	181 (98%)	4 (2%)	52	65
2	E	128/133 (96%)	119 (93%)	9 (7%)	15	16
2	F	119/133 (90%)	110 (92%)	9 (8%)	13	14
2	G	120/133 (90%)	112 (93%)	8 (7%)	16	18
2	H	126/133 (95%)	118 (94%)	8 (6%)	18	20
All	All	1234/1276 (97%)	1181 (96%)	53 (4%)	29	36

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	484	ARG
1	A	507	LYS
1	A	508	ARG
1	A	560	LYS
1	A	571	GLN
1	A	595	VAL
1	A	600	SER
1	A	622	SER
1	A	664	GLU
1	B	508	ARG
1	B	564	THR
1	B	625	GLU
1	C	564	THR
1	C	571	GLN
1	C	604	ASP
1	D	489	ARG
1	D	595	VAL
1	D	620	SER
1	D	672	ARG
2	E	102	LEU
2	E	116	ASN
2	E	119	SER
2	E	130	SER
2	E	132	LYS
2	E	139	ASN
2	E	165	LYS
2	E	235	TYR
2	E	248	ASP
2	F	99	LEU
2	F	107	THR
2	F	111	LEU
2	F	138	PRO
2	F	139	ASN
2	F	157	LEU
2	F	160	LYS
2	F	181	ARG
2	F	235	TYR
2	G	103	VAL
2	G	112	SER
2	G	135	ASP
2	G	139	ASN
2	G	156	ARG

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Mol	Chain	Res	Type
2	G	181	ARG
2	G	197	GLU
2	G	235	TYR
2	H	116	ASN
2	H	129	ASP
2	H	132	LYS
2	H	134	LYS
2	H	135	ASP
2	H	139	ASN
2	H	180	ILE
2	H	235	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	515	ASN
1	A	544	HIS
1	A	563	ASN
1	A	571	GLN
1	A	598	HIS
1	A	670	GLN
1	B	501	GLN
1	B	559	ASN
1	B	598	HIS
1	B	635	HIS
1	B	670	GLN
1	C	510	ASN
1	C	559	ASN
1	C	571	GLN
1	C	598	HIS
1	D	510	ASN
1	D	517	ASN
1	D	670	GLN
2	E	139	ASN
2	E	193	HIS
2	F	139	ASN
2	F	240	HIS
2	G	139	ASN
2	G	193	HIS
2	H	139	ASN
2	H	175	ASN
2	H	215	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	PO4	E	408	-	4,4,4	4.14	1 (25%)	6,6,6	1.26	0
3	PO4	C	402	-	4,4,4	3.76	1 (25%)	6,6,6	1.50	2 (33%)
3	PO4	B	401	-	4,4,4	3.60	1 (25%)	6,6,6	1.27	0
3	PO4	D	405	-	4,4,4	4.18	1 (25%)	6,6,6	1.19	0
3	PO4	E	412	-	4,4,4	4.16	1 (25%)	6,6,6	1.47	1 (16%)
3	PO4	B	406	-	4,4,4	4.16	1 (25%)	6,6,6	1.28	0
3	PO4	A	404	-	4,4,4	4.17	1 (25%)	6,6,6	1.24	0
3	PO4	C	407	-	4,4,4	4.12	1 (25%)	6,6,6	1.21	0
3	PO4	F	410	-	4,4,4	4.20	1 (25%)	6,6,6	1.20	0
3	PO4	A	403	-	4,4,4	3.97	1 (25%)	6,6,6	1.81	2 (33%)
3	PO4	E	411	-	4,4,4	4.14	1 (25%)	6,6,6	1.19	1 (16%)
3	PO4	H	409	-	4,4,4	4.15	1 (25%)	6,6,6	1.30	0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	410	PO4	P-O4	8.28	1.79	1.54
3	D	405	PO4	P-O4	8.23	1.79	1.54
3	E	412	PO4	P-O4	8.23	1.79	1.54
3	H	409	PO4	P-O4	8.21	1.79	1.54
3	B	406	PO4	P-O4	8.21	1.79	1.54
3	A	404	PO4	P-O4	8.16	1.79	1.54
3	E	408	PO4	P-O4	8.14	1.79	1.54
3	E	411	PO4	P-O4	8.14	1.79	1.54
3	C	407	PO4	P-O4	8.09	1.78	1.54
3	A	403	PO4	P-O4	7.83	1.78	1.54
3	C	402	PO4	P-O4	7.34	1.76	1.54
3	B	401	PO4	P-O4	7.08	1.75	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	412	PO4	O3-P-O2	2.58	116.26	107.97
3	A	403	PO4	O4-P-O1	-2.54	101.60	110.89
3	A	403	PO4	O4-P-O2	-2.18	100.98	107.97
3	E	411	PO4	O4-P-O1	-2.13	103.11	110.89
3	C	402	PO4	O4-P-O1	-2.12	103.15	110.89
3	C	402	PO4	O3-P-O2	2.11	114.76	107.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	410	PO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	F	121:PRO	C	122:LEU	N	1.68

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	214/214 (100%)	-0.34	1 (0%) 91 90	21, 30, 43, 54	0
1	B	213/214 (99%)	-0.38	3 (1%) 75 73	24, 32, 45, 61	0
1	C	213/214 (99%)	-0.32	3 (1%) 75 73	24, 32, 45, 58	0
1	D	213/214 (99%)	-0.35	1 (0%) 91 90	24, 33, 44, 58	0
2	E	142/150 (94%)	-0.06	2 (1%) 75 73	35, 43, 52, 62	0
2	F	132/150 (88%)	0.96	18 (13%) 3 2	39, 51, 60, 65	0
2	G	134/150 (89%)	0.36	5 (3%) 41 39	39, 49, 55, 58	0
2	H	140/150 (93%)	0.43	6 (4%) 35 33	44, 54, 62, 64	0
All	All	1401/1456 (96%)	-0.05	39 (2%) 53 51	21, 38, 56, 65	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	127	ARG	7.9
2	F	126	ILE	4.8
2	F	129	ASP	4.7
1	B	507	LYS	4.3
2	F	203	GLY	3.8
2	F	125	VAL	3.7
2	H	126	ILE	3.4
2	E	147	ARG	3.4
2	F	205	ALA	3.3
1	D	508	ARG	3.2
1	B	506	GLY	3.2
2	F	140	TYR	3.1
2	F	128	ARG	3.1
2	H	142	ARG	3.0
2	H	192	TYR	2.9
2	G	140	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
2	F	245	VAL	2.8
2	H	114	TYR	2.7
2	F	123	GLU	2.7
1	A	508	ARG	2.7
2	F	124	GLY	2.6
2	H	129	ASP	2.6
2	F	187	SER	2.6
2	G	114	TYR	2.6
1	C	508	ARG	2.5
2	G	157	LEU	2.4
2	G	125	VAL	2.3
2	F	114	TYR	2.3
2	F	232	TRP	2.3
2	G	122	LEU	2.3
2	F	201	TYR	2.2
1	C	505	VAL	2.2
2	F	134	LYS	2.2
2	E	129	ASP	2.2
1	B	509	LYS	2.2
2	F	119	SER	2.1
1	C	604	ASP	2.1
2	H	122	LEU	2.0
2	F	132	LYS	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 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, 95^{th} 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PO4	F	410	5/5	0.90	0.14	91,91,91,92	0
3	PO4	H	409	5/5	0.93	0.15	76,77,78,78	0
3	PO4	A	404	5/5	0.94	0.08	68,69,69,69	0
3	PO4	D	405	5/5	0.96	0.13	79,79,79,80	0
3	PO4	E	411	5/5	0.96	0.16	70,70,71,72	0
3	PO4	E	408	5/5	0.97	0.23	78,78,79,79	0
3	PO4	E	412	5/5	0.98	0.15	57,58,60,60	0
3	PO4	B	406	5/5	0.98	0.07	75,76,76,76	0
3	PO4	A	403	5/5	0.98	0.10	35,35,37,37	0
3	PO4	B	401	5/5	0.99	0.06	24,26,29,29	0
3	PO4	C	402	5/5	0.99	0.06	29,30,31,32	0
3	PO4	C	407	5/5	0.99	0.11	79,79,79,80	0

6.5 Other polymers (i)

There are no such residues in this entry.