



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 2, 2022 – 12:24 PM EDT

PDB ID : 7RHO
Title : Human IgG1 Fc fragment, hinge-free, expressed in E. coli
Authors : Gallagher, D.T.
Deposited on : 2021-07-18
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) 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 : 2.31.2
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) : 2.31.2

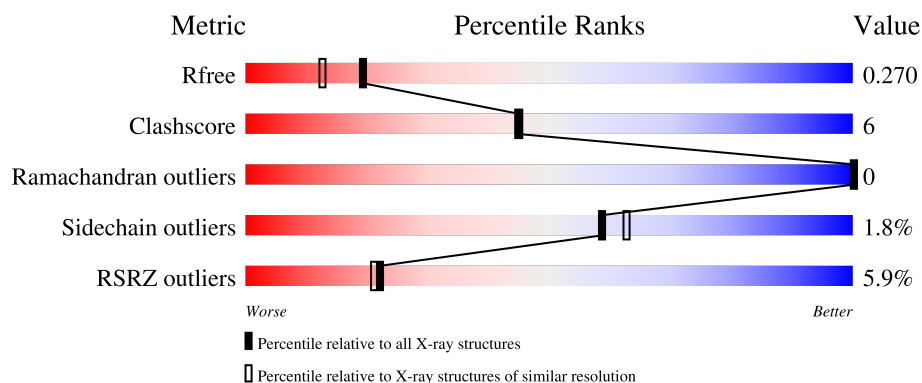
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	213	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div></div> </div> <div>..</div> </div>
1	B	213	<div> <div>4%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div></div> </div> <div>..</div> </div>
1	D	213	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div></div> </div> <div>.</div> </div>
1	E	213	<div> <div>3%</div> <div> <div></div> <div>87%</div> <div>10%</div> <div></div> </div> <div>.</div> </div>
1	F	213	<div> <div>2%</div> <div> <div></div> <div>83%</div> <div>14%</div> <div></div> </div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	213	
1	J	213	
1	K	213	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13842 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 Fc fragment of human IgG1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	0	0	0
			1659	1056	279	317	7			
1	B	206	Total	C	N	O	S	0	0	0
			1651	1052	278	314	7			
1	D	207	Total	C	N	O	S	0	0	0
			1647	1051	274	315	7			
1	E	208	Total	C	N	O	S	0	0	0
			1646	1052	275	312	7			
1	F	207	Total	C	N	O	S	0	0	0
			1652	1052	277	316	7			
1	G	207	Total	C	N	O	S	0	0	0
			1626	1035	271	313	7			
1	J	204	Total	C	N	O	S	0	0	0
			1629	1037	274	311	7			
1	K	206	Total	C	N	O	S	0	0	0
			1638	1043	273	315	7			

There are 16 discrepancies between the modelled and reference sequences:

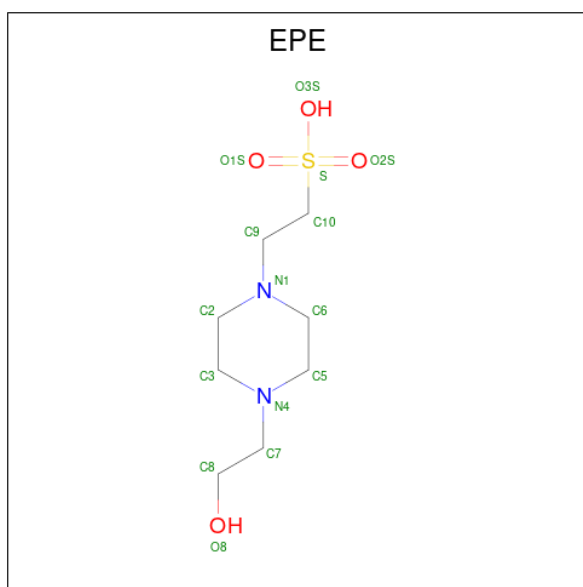
Chain	Residue	Modelled	Actual	Comment	Reference
A	238	MET	-	initiating methionine	UNP Q6MZV7
A	239	ALA	-	expression tag	UNP Q6MZV7
B	238	MET	-	initiating methionine	UNP Q6MZV7
B	239	ALA	-	expression tag	UNP Q6MZV7
D	238	MET	-	initiating methionine	UNP Q6MZV7
D	239	ALA	-	expression tag	UNP Q6MZV7
E	238	MET	-	initiating methionine	UNP Q6MZV7
E	239	ALA	-	expression tag	UNP Q6MZV7
F	238	MET	-	initiating methionine	UNP Q6MZV7
F	239	ALA	-	expression tag	UNP Q6MZV7
G	238	MET	-	initiating methionine	UNP Q6MZV7
G	239	ALA	-	expression tag	UNP Q6MZV7
J	238	MET	-	initiating methionine	UNP Q6MZV7

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Chain	Residue	Modelled	Actual	Comment	Reference
J	239	ALA	-	expression tag	UNP Q6MZV7
K	238	MET	-	initiating methionine	UNP Q6MZV7
K	239	ALA	-	expression tag	UNP Q6MZV7

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	109	Total	O	0	0
			109	109		
3	B	104	Total	O	0	0
			104	104		
3	D	85	Total	O	0	0
			85	85		
3	E	75	Total	O	0	0
			75	75		
3	F	78	Total	O	0	0
			78	78		

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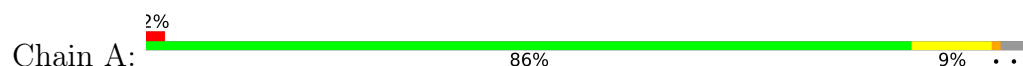
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	92	Total 92	O 92	0	0
3	J	57	Total 57	O 57	0	0
3	K	64	Total 64	O 64	0	0

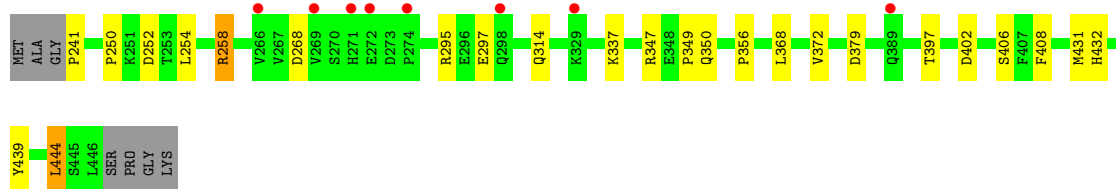
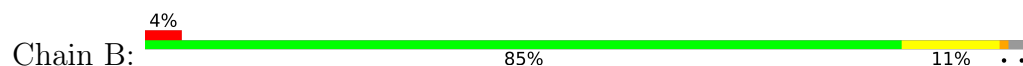
3 Residue-property plots [i](#)

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.

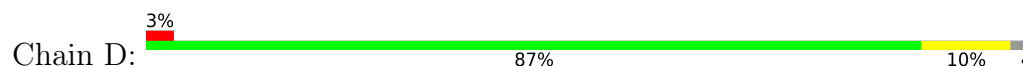
- Molecule 1: Fc fragment of human IgG1



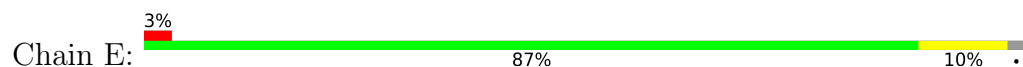
- Molecule 1: Fc fragment of human IgG1



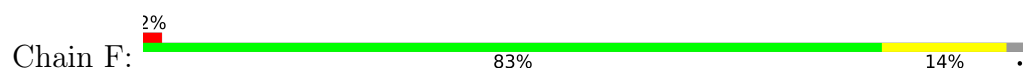
- Molecule 1: Fc fragment of human IgG1

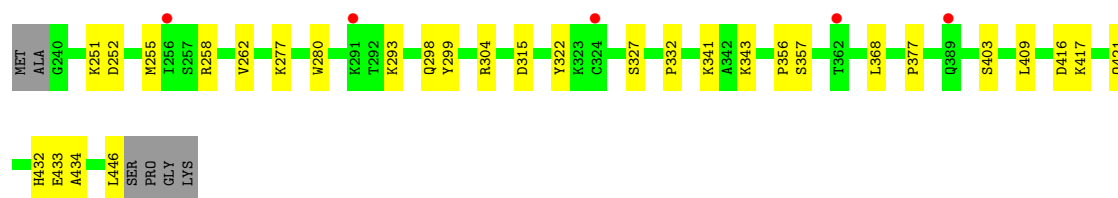


- Molecule 1: Fc fragment of human IgG1

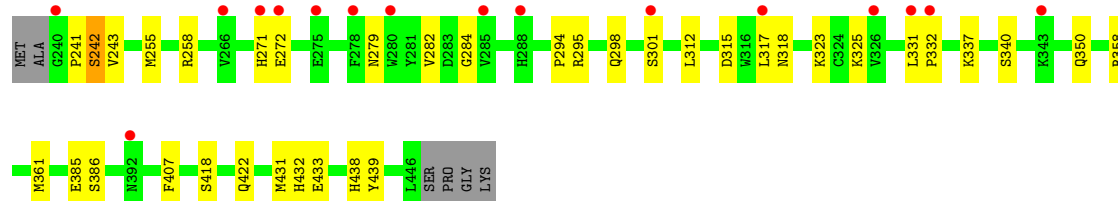
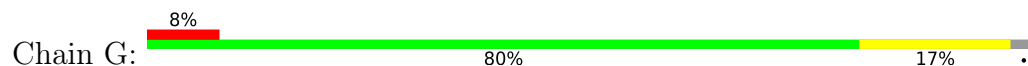


- Molecule 1: Fc fragment of human IgG1

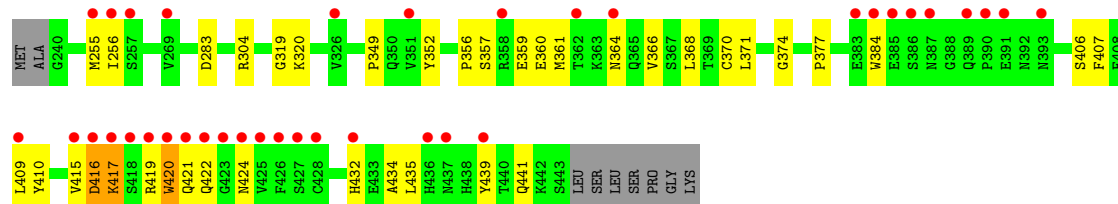
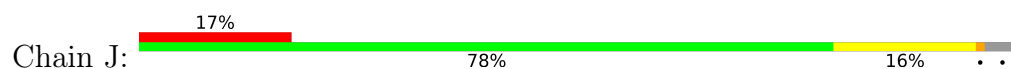




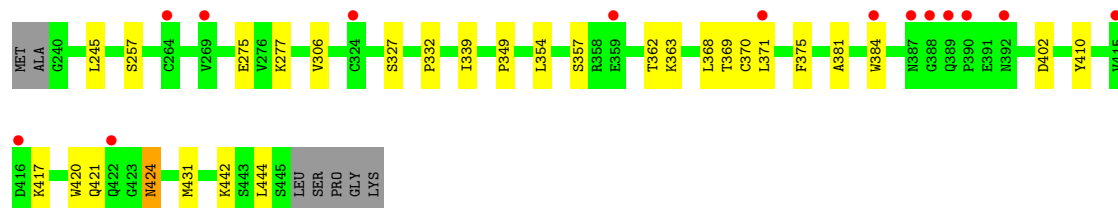
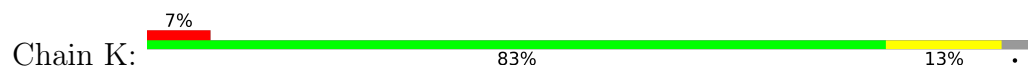
- Molecule 1: Fc fragment of human IgG1



- Molecule 1: Fc fragment of human IgG1



- Molecule 1: Fc fragment of human IgG1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.84Å 150.39Å 241.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.00 14.97 – 2.00	Depositor EDS
% Data completeness (in resolution range)	88.6 (15.00-2.00) 88.8 (14.97-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.220 , 0.270 0.220 , 0.270	Depositor DCC
R_{free} test set	5637 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	42.3	Xtriage
Anisotropy	0.121	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13842	wwPDB-VP
Average B, all atoms (Å ²)	54.0	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 39.27 % 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 3.2529e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPE

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	0.36	0/1705	0.74	0/2322
1	B	0.36	0/1697	0.73	0/2311
1	D	0.39	0/1693	0.72	0/2307
1	E	0.36	0/1692	0.71	0/2306
1	F	0.36	0/1698	0.71	0/2314
1	G	0.37	0/1671	0.74	0/2282
1	J	0.34	0/1675	0.64	0/2282
1	K	0.34	0/1683	0.68	0/2293
All	All	0.36	0/13514	0.71	0/18417

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

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	1659	0	1626	23	0
1	B	1651	0	1620	22	0
1	D	1647	0	1607	24	0
1	E	1646	0	1608	14	0
1	F	1652	0	1611	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1626	0	1562	22	0
1	J	1629	0	1587	35	0
1	K	1638	0	1595	22	0
2	A	15	0	17	0	0
2	F	15	0	17	0	0
3	A	109	0	0	1	0
3	B	104	0	0	9	0
3	D	85	0	0	1	0
3	E	75	0	0	3	0
3	F	78	0	0	1	0
3	G	92	0	0	3	0
3	J	57	0	0	5	0
3	K	64	0	0	0	0
All	All	13842	0	12850	169	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 6.

All (169) 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:B:252:ASP:OD1	1:B:258:ARG:HD3	1.69	0.93
1:J:416:ASP:OD1	1:J:419:ARG:HG3	1.70	0.92
1:D:356:PRO:CG	1:D:366:VAL:CG1	2.49	0.91
1:D:356:PRO:HG2	1:D:366:VAL:HG11	1.57	0.85
1:G:242:SER:HB2	3:G:511:HOH:O	1.77	0.85
1:D:356:PRO:CG	1:D:366:VAL:HG11	2.07	0.84
1:F:432:HIS:HD2	1:F:434:ALA:H	1.25	0.83
1:F:293:LYS:HG2	3:F:1061:HOH:O	1.81	0.81
1:A:268:ASP:HA	1:A:302:THR:HG21	1.62	0.80
1:D:356:PRO:CB	1:D:366:VAL:CG1	2.60	0.80
1:F:432:HIS:CD2	1:F:434:ALA:H	2.01	0.79
1:J:417:LYS:O	1:J:421:GLN:HG3	1.83	0.79
1:D:356:PRO:HG3	1:D:366:VAL:HG12	1.64	0.79
1:A:268:ASP:HA	1:A:302:THR:CG2	2.13	0.78
1:J:439:TYR:OH	1:J:441:GLN:OE1	2.01	0.78
1:E:418:SER:O	1:E:422:GLN:HG3	1.83	0.78
1:G:243:VAL:O	1:G:337:LYS:NZ	2.16	0.77
1:D:356:PRO:HB3	1:D:366:VAL:CG1	2.14	0.77
1:D:356:PRO:CG	1:D:366:VAL:HG12	2.14	0.77
1:J:356:PRO:HB3	1:J:366:VAL:HG22	1.65	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:417:LYS:HE2	3:J:541:HOH:O	1.84	0.77
1:A:255:MET:HE2	1:A:258:ARG:HD2	1.68	0.74
1:F:251:LYS:HG2	1:F:255:MET:HE2	1.69	0.74
1:B:349:PRO:CD	3:B:501:HOH:O	2.36	0.73
1:A:255:MET:CE	1:A:258:ARG:HD2	2.19	0.72
1:J:364:ASN:O	1:J:417:LYS:HB3	1.89	0.72
1:A:252:ASP:OD2	1:A:258:ARG:NH1	2.22	0.71
1:B:241:PRO:HA	1:B:268:ASP:HB2	1.71	0.71
1:B:349:PRO:HD3	3:B:501:HOH:O	1.91	0.71
1:B:432:HIS:ND1	3:B:501:HOH:O	2.25	0.70
1:G:279:ASN:HB2	1:G:325:LYS:HB3	1.74	0.69
1:F:332:PRO:HB3	1:J:407:PHE:CZ	2.28	0.69
1:F:251:LYS:HG2	1:F:255:MET:CE	2.27	0.64
1:B:431:MET:HE2	3:B:550:HOH:O	1.98	0.63
1:K:354:LEU:HB2	1:K:369:THR:HB	1.82	0.61
1:D:432:HIS:CD2	1:D:434:ALA:H	2.17	0.61
1:D:432:HIS:HD2	1:D:434:ALA:H	1.50	0.60
1:K:417:LYS:HG2	1:K:421:GLN:HE21	1.66	0.60
1:E:443:SER:HB2	3:E:571:HOH:O	2.01	0.60
1:J:377:PRO:O	1:J:432:HIS:HE1	1.85	0.59
1:F:298:GLN:HE21	1:F:304:ARG:HH11	1.51	0.59
1:G:350:GLN:HG2	3:G:573:HOH:O	2.00	0.59
1:B:350:GLN:HG3	3:B:509:HOH:O	2.03	0.59
1:B:356:PRO:HD3	1:B:368:LEU:CD2	2.32	0.59
1:D:356:PRO:HB3	1:D:366:VAL:HG13	1.86	0.58
1:J:349:PRO:HG2	1:J:435:LEU:HD21	1.85	0.57
1:G:418:SER:O	1:G:422:GLN:HG3	2.05	0.57
1:B:349:PRO:HD2	3:B:501:HOH:O	2.03	0.57
1:E:288:HIS:CE1	1:G:318:ASN:HB3	2.40	0.57
1:G:331:LEU:HD23	1:G:332:PRO:HD2	1.87	0.57
1:A:397:THR:HG21	1:B:397:THR:HG21	1.87	0.56
1:D:312:LEU:HD23	1:D:312:LEU:N	2.20	0.56
1:J:417:LYS:CE	3:J:541:HOH:O	2.48	0.56
1:J:356:PRO:CB	1:J:366:VAL:HG22	2.34	0.55
1:K:371:LEU:HB2	1:K:410:TYR:CE1	2.42	0.55
1:F:277:LYS:HB3	1:F:327:SER:HB2	1.89	0.55
1:B:297:GLU:O	1:D:304:ARG:NH2	2.41	0.54
1:J:371:LEU:HD13	1:J:410:TYR:CZ	2.42	0.54
1:G:271:HIS:HB2	1:G:301:SER:O	2.08	0.54
1:J:416:ASP:HB3	1:J:419:ARG:HD2	1.90	0.54
1:A:364:ASN:HD21	1:F:416:ASP:CG	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:361:MET:O	1:E:417:LYS:HD3	2.07	0.54
1:J:368:LEU:HD11	1:J:420:TRP:CE3	2.43	0.54
1:F:409:LEU:C	1:F:409:LEU:HD12	2.29	0.53
1:D:262:VAL:HG13	1:D:311:VAL:HG11	1.90	0.53
1:J:356:PRO:HB3	1:J:366:VAL:CG2	2.38	0.53
1:E:337:LYS:HD2	3:E:510:HOH:O	2.09	0.52
1:K:370:CYS:HB2	1:K:384:TRP:CZ2	2.44	0.52
1:A:262:VAL:HG23	1:A:280:TRP:CH2	2.44	0.52
1:F:377:PRO:O	1:F:432:HIS:HE1	1.93	0.52
1:B:337:LYS:HE3	3:B:594:HOH:O	2.09	0.52
1:K:277:LYS:HB3	1:K:327:SER:HB2	1.91	0.52
1:J:432:HIS:CD2	1:J:434:ALA:H	2.29	0.51
1:G:358:ARG:O	1:G:361:MET:HB2	2.10	0.51
1:G:298:GLN:HA	1:J:304:ARG:HH22	1.75	0.51
1:K:424:ASN:H	1:K:424:ASN:HD22	1.59	0.51
1:G:241:PRO:HG2	1:G:331:LEU:HG	1.93	0.50
1:J:356:PRO:HD2	1:J:420:TRP:CZ2	2.46	0.50
1:A:268:ASP:HA	1:A:302:THR:HG23	1.92	0.50
1:B:314:GLN:HG3	3:B:563:HOH:O	2.11	0.50
1:E:417:LYS:HD2	1:E:421:GLN:NE2	2.25	0.50
1:F:417:LYS:HE2	1:F:421:GLN:CD	2.32	0.50
1:J:319:GLY:HA2	3:J:515:HOH:O	2.12	0.50
1:F:252:ASP:OD2	1:F:258:ARG:NH1	2.44	0.49
1:D:377:PRO:O	1:D:432:HIS:HE1	1.94	0.49
1:G:323:LYS:HA	1:G:337:LYS:O	2.13	0.49
1:E:323:LYS:HG3	1:E:338:THR:OG1	2.13	0.49
1:K:349:PRO:HB3	1:K:375:PHE:HB3	1.96	0.48
1:K:362:THR:HB	1:K:363:LYS:HD2	1.95	0.48
1:K:245:LEU:HD23	1:K:339:ILE:HG23	1.95	0.48
1:J:361:MET:O	1:J:417:LYS:HE3	2.12	0.48
1:D:397:THR:HG21	1:E:397:THR:HG21	1.95	0.48
1:G:312:LEU:HB2	1:G:315:ASP:HB2	1.95	0.48
1:J:361:MET:O	1:J:417:LYS:CE	2.62	0.47
1:B:444:LEU:N	1:B:444:LEU:HD12	2.29	0.47
1:J:409:LEU:C	1:J:409:LEU:HD12	2.35	0.47
1:A:262:VAL:HG23	1:A:280:TRP:CZ3	2.50	0.47
1:G:317:LEU:HG	3:G:545:HOH:O	2.15	0.47
1:D:267:VAL:HG12	1:D:304:ARG:HD2	1.97	0.47
1:D:409:LEU:HD12	1:D:409:LEU:C	2.35	0.47
1:K:354:LEU:HD12	1:K:369:THR:CG2	2.45	0.46
1:E:353:THR:HB	1:E:444:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:PRO:CB	1:D:366:VAL:HG12	2.42	0.46
1:F:332:PRO:HB3	1:J:407:PHE:HZ	1.78	0.46
1:G:385:GLU:HG2	1:G:386:SER:N	2.30	0.46
1:K:424:ASN:HD22	1:K:424:ASN:N	2.14	0.46
1:K:417:LYS:HG2	1:K:421:GLN:NE2	2.29	0.46
1:D:445:SER:O	1:D:446:LEU:C	2.54	0.46
1:E:241:PRO:HG2	1:E:331:LEU:HG	1.97	0.46
1:B:372:VAL:O	1:B:408:PHE:HA	2.16	0.45
1:A:446:LEU:C	1:A:446:LEU:HD23	2.36	0.45
1:E:274:PRO:HD2	1:E:275:GLU:OE1	2.15	0.45
1:D:356:PRO:CB	1:D:366:VAL:HG11	2.40	0.45
1:K:417:LYS:HB3	1:K:417:LYS:HE2	1.58	0.45
1:A:332:PRO:HB3	1:D:407:PHE:CZ	2.52	0.45
1:B:254:LEU:HD22	3:B:593:HOH:O	2.16	0.45
1:F:332:PRO:HB2	3:J:537:HOH:O	2.17	0.45
1:B:444:LEU:HD12	1:B:444:LEU:H	1.81	0.44
1:F:421:GLN:HA	1:F:446:LEU:HD12	2.00	0.44
1:J:283:ASP:OD2	1:J:320:LYS:HG2	2.18	0.43
1:J:432:HIS:HD2	1:J:434:ALA:H	1.66	0.43
1:A:299:TYR:CE2	1:E:306:VAL:HG21	2.53	0.43
1:F:341:LYS:HE3	1:F:433:GLU:OE2	2.19	0.43
1:F:299:TYR:CE2	1:K:306:VAL:HG21	2.53	0.43
1:A:389:GLN:HE21	1:A:389:GLN:HB2	1.49	0.43
1:A:255:MET:HE3	1:A:258:ARG:HD2	1.99	0.43
1:A:436:HIS:HB3	3:A:1064:HOH:O	2.19	0.43
1:B:356:PRO:HD3	1:B:368:LEU:HD23	1.99	0.43
1:J:374:GLY:HA2	1:J:406:SER:OG	2.19	0.43
1:J:415:VAL:HG12	3:J:546:HOH:O	2.17	0.43
1:G:432:HIS:O	1:G:438:HIS:HA	2.19	0.43
1:J:419:ARG:HA	1:J:422:GLN:HE21	1.83	0.43
1:G:282:VAL:C	1:G:284:GLY:H	2.22	0.43
1:G:255:MET:HB2	1:G:258:ARG:HD2	2.01	0.42
1:J:357:SER:OG	1:K:354:LEU:HD23	2.19	0.42
1:A:332:PRO:HB2	3:D:543:HOH:O	2.19	0.42
1:J:360:GLU:HG2	1:J:366:VAL:HG23	2.01	0.42
1:K:420:TRP:CH2	1:K:444:LEU:HG	2.55	0.42
1:B:347:ARG:NH2	1:B:406:SER:HB3	2.35	0.42
1:J:359:GLU:OE1	1:K:442:LYS:HE3	2.19	0.42
1:A:322:TYR:O	1:A:338:THR:HA	2.19	0.42
1:A:345:GLN:HE21	1:A:345:GLN:HB2	1.61	0.42
1:A:409:LEU:C	1:A:409:LEU:HD12	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:262:VAL:HG23	1:F:280:TRP:CH2	2.55	0.42
1:K:381:ALA:HB3	1:K:431:MET:HB2	2.00	0.42
1:A:298:GLN:NE2	1:A:304:ARG:HB2	2.34	0.42
1:G:433:GLU:O	1:G:438:HIS:HD2	2.02	0.42
1:J:422:GLN:HB2	1:J:424:ASN:ND2	2.35	0.42
1:K:368:LEU:HD13	1:K:444:LEU:HD23	2.02	0.42
1:E:417:LYS:HB3	1:E:417:LYS:HE2	1.85	0.41
1:K:354:LEU:HD12	1:K:369:THR:HG21	2.02	0.41
1:G:431:MET:HG2	1:G:439:TYR:CD2	2.55	0.41
1:J:255:MET:HG3	1:J:256:ILE:H	1.85	0.41
1:J:352:TYR:HB3	1:K:357:SER:HB3	2.02	0.41
1:D:371:LEU:HD13	1:D:410:TYR:CZ	2.55	0.41
1:J:370:CYS:HB2	1:J:384:TRP:CZ2	2.55	0.41
1:A:361:MET:O	1:A:417:LYS:HE3	2.21	0.41
1:G:407:PHE:HZ	1:K:332:PRO:HB3	1.86	0.41
1:A:298:GLN:OE1	1:A:302:THR:HG22	2.21	0.41
1:B:356:PRO:HD3	1:B:368:LEU:HD22	2.02	0.41
1:B:431:MET:HG2	1:B:439:TYR:CD2	2.56	0.41
1:E:239:ALA:HA	3:E:567:HOH:O	2.21	0.41
1:F:341:LYS:CE	1:F:433:GLU:OE2	2.68	0.41
1:G:294:PRO:O	1:G:295:ARG:C	2.58	0.41
1:F:315:ASP:HB3	1:F:322:TYR:OH	2.22	0.40
1:F:356:PRO:HD3	1:F:368:LEU:HD12	2.04	0.40
1:D:378:SER:HB3	1:D:407:PHE:CE1	2.56	0.40
1:B:250:PRO:HB3	1:B:379:ASP:HB3	2.04	0.40
1:D:415:VAL:HG11	1:D:426:PHE:CE2	2.56	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	205/213 (96%)	202 (98%)	3 (2%)	0	100	100
1	B	204/213 (96%)	199 (98%)	5 (2%)	0	100	100
1	D	205/213 (96%)	202 (98%)	3 (2%)	0	100	100
1	E	206/213 (97%)	201 (98%)	5 (2%)	0	100	100
1	F	205/213 (96%)	200 (98%)	5 (2%)	0	100	100
1	G	205/213 (96%)	196 (96%)	9 (4%)	0	100	100
1	J	202/213 (95%)	194 (96%)	8 (4%)	0	100	100
1	K	204/213 (96%)	201 (98%)	3 (2%)	0	100	100
All	All	1636/1704 (96%)	1595 (98%)	41 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	193/197 (98%)	189 (98%)	4 (2%)	53	57
1	B	192/197 (98%)	188 (98%)	4 (2%)	53	57
1	D	190/197 (96%)	187 (98%)	3 (2%)	62	67
1	E	188/197 (95%)	185 (98%)	3 (2%)	62	67
1	F	191/197 (97%)	188 (98%)	3 (2%)	62	67
1	G	185/197 (94%)	182 (98%)	3 (2%)	62	67
1	J	188/197 (95%)	185 (98%)	3 (2%)	62	67
1	K	189/197 (96%)	185 (98%)	4 (2%)	53	57
All	All	1516/1576 (96%)	1489 (98%)	27 (2%)	59	63

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	302	THR
1	A	345	GLN

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Mol	Chain	Res	Type
1	A	389	GLN
1	A	443	SER
1	B	258	ARG
1	B	295	ARG
1	B	402	ASP
1	B	444	LEU
1	D	256	ILE
1	D	429	SER
1	D	445	SER
1	E	259	THR
1	E	295	ARG
1	E	445	SER
1	F	343	LYS
1	F	357	SER
1	F	403	SER
1	G	242	SER
1	G	272	GLU
1	G	340	SER
1	J	416	ASP
1	J	417	LYS
1	J	420	TRP
1	K	257	SER
1	K	275	GLU
1	K	402	ASP
1	K	424	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	345	GLN
1	A	364	ASN
1	A	389	GLN
1	A	421	GLN
1	A	437	ASN
1	B	437	ASN
1	D	387	ASN
1	D	389	GLN
1	D	424	ASN
1	D	432	HIS
1	E	288	HIS
1	E	350	GLN
1	E	421	GLN

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Mol	Chain	Res	Type
1	F	298	GLN
1	F	432	HIS
1	G	279	ASN
1	G	421	GLN
1	G	436	HIS
1	G	437	ASN
1	G	438	HIS
1	J	271	HIS
1	J	365	GLN
1	J	422	GLN
1	J	424	ASN
1	J	432	HIS
1	J	436	HIS
1	J	437	ASN
1	K	364	ASN
1	K	389	GLN
1	K	421	GLN
1	K	424	ASN

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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	EPE	F	900	-	15,15,15	0.80	1 (6%)	18,20,20	0.89	2 (11%)
2	EPE	A	900	-	15,15,15	1.05	1 (6%)	18,20,20	1.45	2 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EPE	F	900	-	-	3/9/19/19	0/1/1/1
2	EPE	A	900	-	-	7/9/19/19	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	EPE	O1S-S	3.80	1.56	1.45
2	F	900	EPE	O1S-S	2.74	1.53	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	EPE	O1S-S-C10	-4.35	101.67	106.92
2	A	900	EPE	O3S-S-O2S	3.69	120.28	111.27
2	F	900	EPE	O1S-S-C10	-2.30	104.14	106.92
2	F	900	EPE	O3S-S-O2S	2.19	116.61	111.27

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	EPE	C9-C10-S-O2S
2	F	900	EPE	N4-C7-C8-O8
2	A	900	EPE	C10-C9-N1-C2
2	A	900	EPE	C10-C9-N1-C6
2	A	900	EPE	C9-C10-S-O3S
2	A	900	EPE	C9-C10-S-O1S
2	A	900	EPE	C8-C7-N4-C3

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Mol	Chain	Res	Type	Atoms
2	F	900	EPE	C10-C9-N1-C2
2	F	900	EPE	C10-C9-N1-C6
2	A	900	EPE	C8-C7-N4-C5

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	207/213 (97%)	0.05	4 (1%) 66 65	29, 46, 64, 75	0
1	B	206/213 (96%)	0.20	8 (3%) 39 38	31, 48, 81, 95	0
1	D	207/213 (97%)	0.09	7 (3%) 45 44	33, 45, 70, 94	0
1	E	208/213 (97%)	0.18	7 (3%) 45 44	35, 49, 69, 82	0
1	F	207/213 (97%)	0.09	5 (2%) 59 57	30, 50, 69, 81	0
1	G	207/213 (97%)	0.33	16 (7%) 13 12	29, 51, 79, 104	0
1	J	204/213 (95%)	0.82	37 (18%) 1 1	41, 64, 125, 137	0
1	K	206/213 (96%)	0.44	14 (6%) 17 16	36, 55, 90, 102	0
All	All	1652/1704 (96%)	0.27	98 (5%) 22 21	29, 51, 86, 137	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	423	GLY	7.9
1	J	385	GLU	5.9
1	J	418	SER	5.9
1	J	389	GLN	5.7
1	J	384	TRP	5.6
1	K	388	GLY	5.6
1	J	256	ILE	5.2
1	J	419	ARG	5.1
1	E	239	ALA	5.0
1	J	358	ARG	5.0
1	J	420	TRP	4.4
1	J	390	PRO	4.2
1	J	416	ASP	3.6
1	G	240	GLY	3.6
1	D	446	LEU	3.5
1	J	422	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	J	428	CYS	3.4
1	K	392	ASN	3.1
1	G	285	VAL	3.1
1	K	389	GLN	3.0
1	F	362	THR	3.0
1	D	256	ILE	2.9
1	D	436	HIS	2.9
1	J	386	SER	2.9
1	G	343	LYS	2.9
1	K	324	CYS	2.9
1	J	351	VAL	2.8
1	G	392	ASN	2.8
1	F	256	ILE	2.8
1	J	421	GLN	2.8
1	J	257	SER	2.8
1	J	427	SER	2.8
1	A	253	THR	2.8
1	J	439	TYR	2.8
1	G	271	HIS	2.7
1	G	266	VAL	2.7
1	K	390	PRO	2.7
1	K	371	LEU	2.7
1	K	269	VAL	2.6
1	K	359	GLU	2.6
1	J	391	GLU	2.6
1	J	436	HIS	2.6
1	J	269	VAL	2.6
1	B	329	LYS	2.6
1	F	291	LYS	2.6
1	J	364	ASN	2.6
1	G	288	HIS	2.6
1	J	432	HIS	2.6
1	D	389	GLN	2.6
1	J	437	ASN	2.6
1	B	269	VAL	2.6
1	G	317	LEU	2.6
1	B	274	PRO	2.5
1	E	392	ASN	2.5
1	G	326	VAL	2.5
1	B	272	GLU	2.5
1	A	389	GLN	2.4
1	J	326	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	255	MET	2.4
1	K	387	ASN	2.4
1	J	417	LYS	2.4
1	F	324	CYS	2.4
1	B	266	VAL	2.4
1	D	326	VAL	2.4
1	A	358	ARG	2.3
1	J	409	LEU	2.3
1	D	388	GLY	2.3
1	G	301	SER	2.3
1	K	416	ASP	2.3
1	K	422	GLN	2.3
1	J	426	PHE	2.3
1	J	383	GLU	2.3
1	J	387	ASN	2.3
1	G	272	GLU	2.3
1	G	275	GLU	2.3
1	K	415	VAL	2.3
1	K	264	CYS	2.3
1	G	278	PHE	2.2
1	B	271	HIS	2.2
1	E	384	TRP	2.2
1	G	331	LEU	2.2
1	E	280	TRP	2.2
1	G	280	TRP	2.2
1	E	257	SER	2.2
1	B	298	GLN	2.1
1	D	422	GLN	2.1
1	K	384	TRP	2.1
1	J	362	THR	2.1
1	A	254	LEU	2.1
1	J	393	ASN	2.1
1	J	424	ASN	2.1
1	E	389	GLN	2.1
1	E	385	GLU	2.1
1	J	415	VAL	2.1
1	J	425	VAL	2.0
1	F	389	GLN	2.0
1	B	389	GLN	2.0
1	G	332	PRO	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, 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(\AA^2)	Q<0.9
2	EPE	A	900	15/15	0.92	0.17	61,73,91,94	0
2	EPE	F	900	15/15	0.92	0.17	64,77,79,81	0

6.5 Other polymers [i](#)

There are no such residues in this entry.