Full wwPDB X-ray Structure Validation Report (i)

Nov 4, 2026 – 02:14 PM JST

PDB ID	:	44JA / pdb_000044ja
Title	:	KIR2DS1 bound to HLA-C*05:01 presenting the P2-AV peptide
Authors	:	Faoro, C.; Rossjohn, J.
Deposited on	:	2026-07-31
Resolution	:	2.95 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:

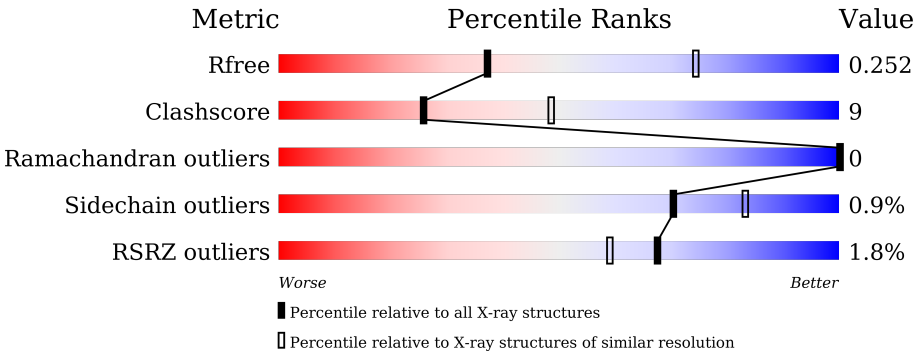
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 2.95 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.



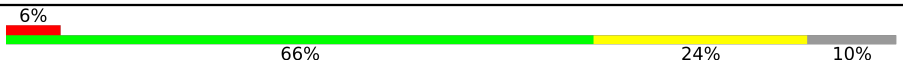
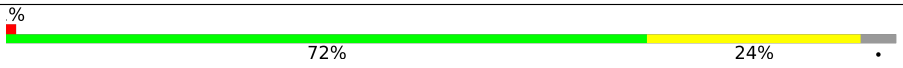
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	279	80% 18%
1	E	279	78% 21%
2	B	100	80% 20%
2	F	100	77% 23%
3	C	9	67% 33%
3	G	9	67% 33%

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Mol	Chain	Length	Quality of chain
4	D	204	
4	H	204	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9334 atoms, of which 91 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 HLA class I histocompatibility antigen, C alpha chain.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	275	Total C H N O S 2235 1389 12 411 415 8	0	0	0
1	E	275	Total C N O S 2250 1404 416 422 8	0	1	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP P10321
A	1	MET	-	expression tag	UNP P10321
A	9	TYR	ASP	variant	UNP P10321
A	24	ALA	SER	variant	UNP P10321
A	35	GLN	ARG	variant	UNP P10321
A	73	THR	ALA	variant	UNP P10321
A	77	ASN	SER	variant	UNP P10321
A	80	LYS	ASN	variant	UNP P10321
A	90	ALA	ASP	variant	UNP P10321
A	99	TYR	SER	variant	UNP P10321
A	114	ASN	ASP	variant	UNP P10321
A	116	PHE	SER	variant	UNP P10321
A	138	LYS	THR	variant	UNP P10321
A	147	TRP	LEU	variant	UNP P10321
A	152	GLU	ALA	variant	UNP P10321
A	156	ARG	LEU	variant	UNP P10321
A	177	LYS	GLU	variant	UNP P10321
A	184	HIS	PRO	variant	UNP P10321
A	194	VAL	LEU	variant	UNP P10321
A	253	GLU	GLN	variant	UNP P10321
A	261	VAL	MET	variant	UNP P10321
A	267	PRO	GLN	variant	UNP P10321
A	273	ARG	SER	variant	UNP P10321
A	275	GLY	GLU	variant	UNP P10321
E	0	MET	-	initiating methionine	UNP P10321

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1	MET	-	expression tag	UNP P10321
E	9	TYR	ASP	variant	UNP P10321
E	24	ALA	SER	variant	UNP P10321
E	35	GLN	ARG	variant	UNP P10321
E	73	THR	ALA	variant	UNP P10321
E	77	ASN	SER	variant	UNP P10321
E	80	LYS	ASN	variant	UNP P10321
E	90	ALA	ASP	variant	UNP P10321
E	99	TYR	SER	variant	UNP P10321
E	114	ASN	ASP	variant	UNP P10321
E	116	PHE	SER	variant	UNP P10321
E	138	LYS	THR	variant	UNP P10321
E	147	TRP	LEU	variant	UNP P10321
E	152	GLU	ALA	variant	UNP P10321
E	156	ARG	LEU	variant	UNP P10321
E	177	LYS	GLU	variant	UNP P10321
E	184	HIS	PRO	variant	UNP P10321
E	194	VAL	LEU	variant	UNP P10321
E	253	GLU	GLN	variant	UNP P10321
E	261	VAL	MET	variant	UNP P10321
E	267	PRO	GLN	variant	UNP P10321
E	273	ARG	SER	variant	UNP P10321
E	275	GLY	GLU	variant	UNP P10321

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	B	100	Total C H N O S 904 525 79 139 157 4	0	0	0
2	F	100	Total C N O S 825 526 140 156 3	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	initiating methionine	UNP P61769
F	0	MET	-	initiating methionine	UNP P61769

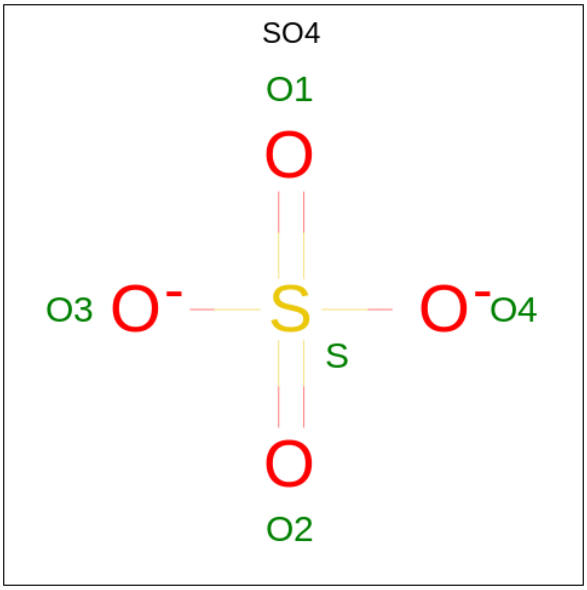
- Molecule 3 is a protein called P2-AV peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	9	Total 63	C 40	N 10	O 13	0	0	0
3	G	9	Total 63	C 40	N 10	O 13	0	0	0

- Molecule 4 is a protein called Killer cell immunoglobulin-like receptor 2DS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	183	Total 1374	C 862	N 244	O 261	S 7	0	0	0
4	H	195	Total 1511	C 952	N 267	O 284	S 8	0	0	0

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 5	O 4	S 1	0	0
5	A	1	Total 5	O 4	S 1	0	0
5	A	1	Total 5	O 4	S 1	0	0
5	B	1	Total 5	O 4	S 1	0	0
5	B	1	Total 5	O 4	S 1	0	0
5	E	1	Total 5	O 4	S 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	1	Total O S 5 4 1	0	0
5	E	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	F	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	D	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0
5	H	1	Total O S 5 4 1	0	0

- Molecule 6 is water.

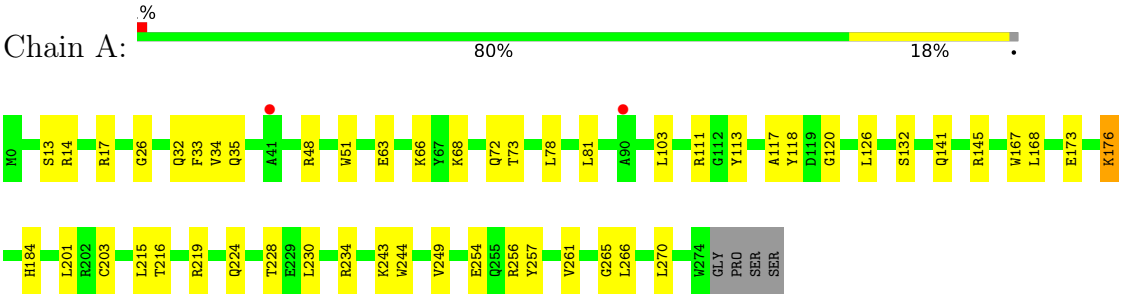
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	3	Total O 3 3	0	0
6	B	2	Total O 2 2	0	0
6	C	1	Total O 1 1	0	0
6	E	5	Total O 5 5	0	0
6	F	6	Total O 6 6	0	0
6	D	5	Total O 5 5	0	0
6	H	2	Total O 2 2	0	0

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.

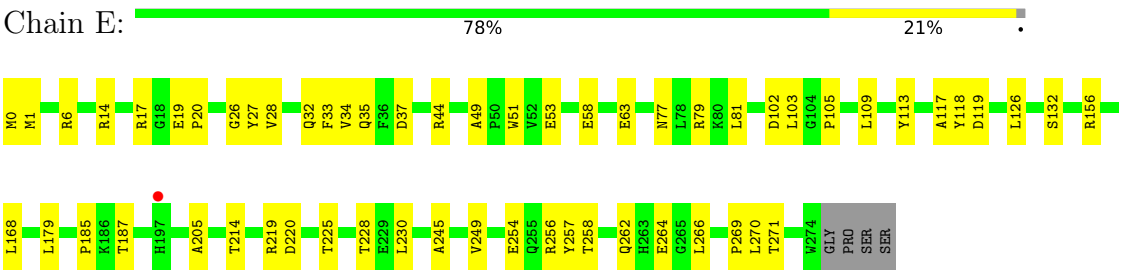
• Molecule 1: HLA class I histocompatibility antigen, C alpha chain

Chain A:



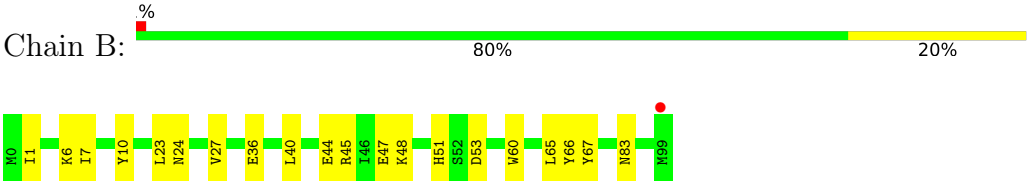
• Molecule 1: HLA class I histocompatibility antigen, C alpha chain

Chain E:



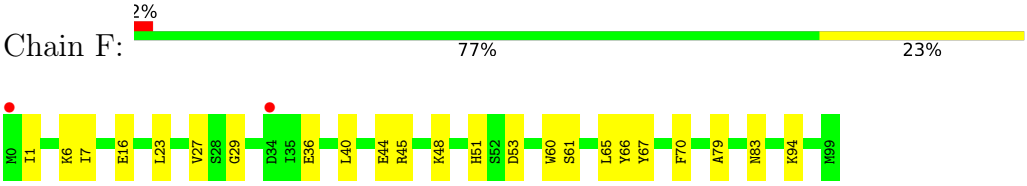
• Molecule 2: Beta-2-microglobulin

Chain B:



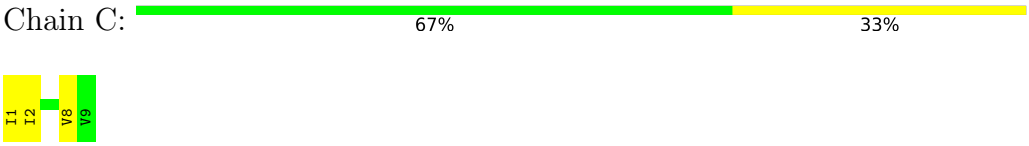
• Molecule 2: Beta-2-microglobulin

Chain F:



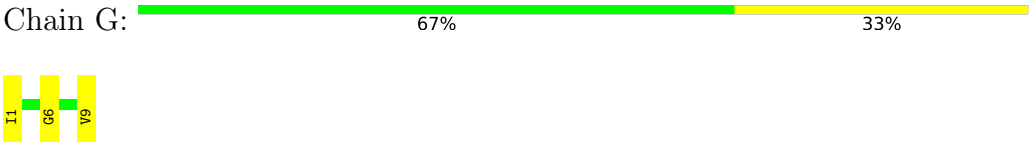
• Molecule 3: P2-AV peptide

Chain C:



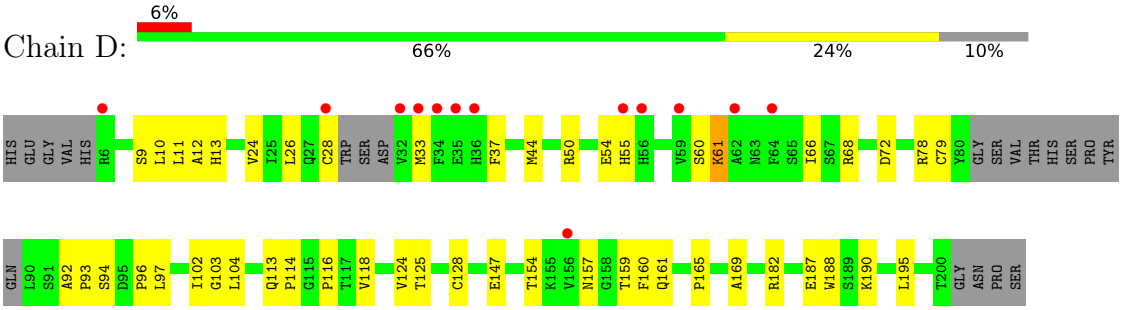
• Molecule 3: P2-AV peptide

Chain G:



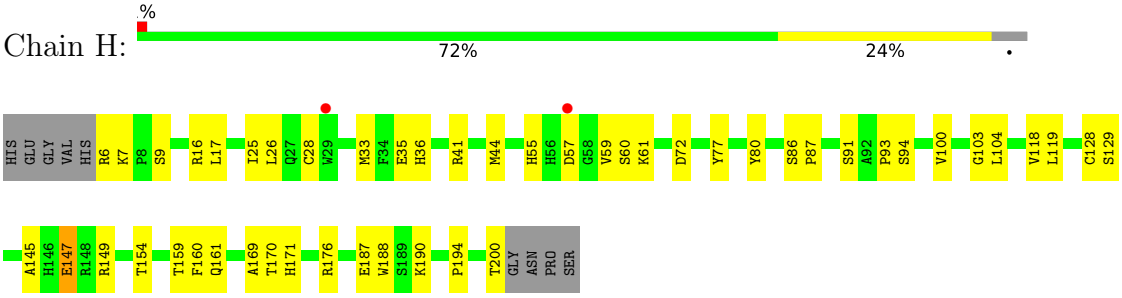
• Molecule 4: Killer cell immunoglobulin-like receptor 2DS1

Chain D:



• Molecule 4: Killer cell immunoglobulin-like receptor 2DS1

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	69.65Å 93.38Å 230.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.01 – 2.95 49.01 – 2.95	Depositor EDS
% Data completeness (in resolution range)	97.4 (49.01-2.95) 97.3 (49.01-2.95)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.22 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5058	Depositor
R, R_{free}	0.197 , 0.253 0.197 , 0.252	Depositor DCC
R_{free} test set	1580 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å^2)	48.4	Xtriage
Anisotropy	0.923	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 54.3	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	0.93	EDS
Total number of atoms	9334	wwPDB-VP
Average B, all atoms (Å^2)	53.0	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 36.38 % 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 5.0435e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.24	0/2285	0.39	0/3105
1	E	0.25	0/2312	0.40	0/3138
2	B	0.24	0/848	0.41	0/1149
2	F	0.26	0/848	0.43	0/1150
3	C	0.28	0/62	0.38	0/81
3	G	0.33	0/62	0.55	0/81
4	D	0.24	0/1406	0.41	0/1906
4	H	0.25	0/1552	0.42	0/2106
All	All	0.25	0/9375	0.41	0/12716

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	2223	12	2072	35	0
1	E	2250	0	2111	42	0
2	B	825	79	777	16	0
2	F	825	0	781	14	0
3	C	63	0	72	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	63	0	72	4	0
4	D	1374	0	1297	33	0
4	H	1511	0	1455	36	0
5	A	15	0	0	0	0
5	B	10	0	0	0	0
5	D	15	0	0	0	0
5	E	15	0	0	0	0
5	F	15	0	0	0	0
5	H	15	0	0	2	0
6	A	3	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	5	0	0	0	0
6	E	5	0	0	0	0
6	F	6	0	0	1	0
6	H	2	0	0	0	0
All	All	9243	91	8637	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 9.

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)
4:H:33:MET:HA	4:H:33:MET:HE2	1.63	0.80
4:D:79:CYS:H	4:D:94:SER:HB3	1.46	0.78
2:F:44:GLU:N	2:F:44:GLU:OE1	2.18	0.75
1:E:258:THR:CG2	1:E:271:THR:HG23	2.19	0.72
4:H:57:ASP:O	4:H:59:VAL:HG23	1.91	0.70
4:H:176:ARG:CZ	4:H:194:PRO:HG3	2.21	0.70
1:E:1:MET:HG2	1:E:264:GLU:OE2	1.94	0.68
2:B:44:GLU:N	2:B:44:GLU:OE1	2.26	0.67
4:H:104:LEU:HD12	4:H:187:GLU:HB3	1.76	0.67
1:E:225:THR:O	1:E:228:THR:HG22	1.94	0.66
1:A:173:GLU:OE1	1:A:176:LYS:NZ	2.28	0.65
4:D:55:HIS:CE1	4:D:60:SER:HA	2.32	0.65
4:D:103:GLY:HA2	4:D:190:LYS:HG3	1.78	0.64
1:A:35:GLN:HG3	2:B:53:ASP:CG	2.23	0.63
1:A:230:LEU:HD22	1:A:243:LYS:HE3	1.80	0.63
4:D:10:LEU:HG	4:D:97:LEU:HD22	1.79	0.63
4:D:154:THR:HG22	4:D:160:PHE:CE2	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:157:ASN:OD1	4:D:159:THR:HG22	2.00	0.62
1:E:6:ARG:HD2	1:E:113:TYR:OH	2.01	0.60
4:H:55:HIS:HA	4:H:59:VAL:O	2.00	0.60
1:A:224:GLN:O	1:A:228:THR:HG22	2.01	0.60
4:D:92:ALA:HB1	4:D:93:PRO:HD2	1.83	0.59
1:A:215:LEU:CD2	1:A:261:VAL:HG22	2.33	0.59
1:A:126:LEU:HD12	1:A:132:SER:O	2.02	0.59
1:E:19:GLU:HB3	1:E:20:PRO:HD2	1.85	0.59
2:F:36:GLU:HB3	2:F:83:ASN:HB3	1.84	0.59
4:H:33:MET:HE1	4:H:59:VAL:C	2.26	0.59
1:E:44:ARG:HB3	1:E:44:ARG:NH1	2.17	0.58
2:B:36:GLU:HB3	2:B:83:ASN:HB3	1.84	0.58
4:D:104:LEU:HD12	4:D:187:GLU:HB3	1.84	0.58
1:A:14:ARG:HB3	1:A:17:ARG:HB2	1.86	0.57
4:H:33:MET:HE2	4:H:33:MET:CA	2.33	0.57
4:D:116:PRO:HB3	4:D:195:LEU:HD11	1.86	0.57
4:D:9:SER:O	4:D:28:CYS:HA	2.05	0.57
4:D:44:MET:HE3	4:D:72:ASP:HA	1.86	0.56
2:B:40:LEU:HD23	2:B:45:ARG:HA	1.86	0.56
1:A:266:LEU:HD13	1:A:270:LEU:HG	1.86	0.56
2:F:40:LEU:HD23	2:F:45:ARG:HA	1.89	0.55
1:E:81:LEU:HD13	1:E:118:TYR:CD1	2.42	0.55
4:D:125:THR:HG22	4:D:165:PRO:HA	1.88	0.54
4:D:33:MET:HA	4:D:60:SER:HB3	1.89	0.54
1:E:185:PRO:HD2	1:E:266:LEU:HD21	1.90	0.54
2:B:7:ILE:HG12	2:B:27:VAL:HG12	1.89	0.54
4:D:78:ARG:NH2	4:D:96:PRO:HG3	2.23	0.53
4:H:33:MET:HE1	4:H:59:VAL:CA	2.37	0.53
4:H:154:THR:HG22	4:H:160:PHE:CE2	2.43	0.53
2:B:6:LYS:O	2:B:27:VAL:HA	2.08	0.53
1:E:119:ASP:O	2:F:1:ILE:HG22	2.08	0.53
4:D:12:ALA:HB2	4:D:97:LEU:HD21	1.89	0.53
4:D:114:PRO:HD2	4:D:118:VAL:HG12	1.89	0.53
4:D:44:MET:CE	4:D:72:ASP:HA	2.38	0.53
4:H:103:GLY:HA2	4:H:190:LYS:HG3	1.89	0.52
1:E:6:ARG:CD	1:E:113:TYR:OH	2.58	0.52
1:E:77:ASN:OD1	3:G:9:VAL:HG12	2.09	0.52
4:H:80:TYR:CE2	4:H:93:PRO:HB3	2.45	0.52
1:A:120:GLY:HA3	2:B:1:ILE:HD11	1.91	0.52
1:A:81:LEU:HD13	1:A:118:TYR:CD1	2.46	0.51
2:B:1:ILE:HG13	2:B:1:ILE:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:249:VAL:HG12	1:E:257:TYR:CZ	2.46	0.51
4:D:37:PHE:O	4:D:50:ARG:HA	2.11	0.51
1:E:187:THR:HG22	1:E:205:ALA:HA	1.94	0.50
1:A:111:ARG:HG2	1:A:113:TYR:CZ	2.47	0.50
1:E:102:ASP:O	1:E:109:LEU:HD12	2.12	0.50
4:D:114:PRO:HD2	4:D:118:VAL:CG1	2.41	0.50
4:H:55:HIS:CD2	4:H:60:SER:HB3	2.47	0.50
1:E:156:ARG:HH21	3:G:6:GLY:HA3	1.77	0.50
2:F:7:ILE:HG12	2:F:27:VAL:HG12	1.93	0.50
4:D:103:GLY:HA2	4:D:190:LYS:CG	2.42	0.50
1:E:35:GLN:HG3	2:F:53:ASP:CG	2.37	0.49
4:D:118:VAL:HG21	4:D:169:ALA:HB2	1.94	0.49
4:D:128:CYS:O	4:D:161:GLN:HA	2.12	0.49
4:H:17:LEU:HD23	4:H:100:VAL:HB	1.93	0.49
1:A:63:GLU:OE2	3:C:1:ILE:CD1	2.61	0.49
1:A:33:PHE:HB3	1:A:51:TRP:CH2	2.47	0.49
1:A:66:LYS:HE3	3:C:2:ILE:HG22	1.95	0.48
1:A:32:GLN:NE2	1:A:48:ARG:HG3	2.28	0.48
1:A:219:ARG:HD3	1:A:256:ARG:NH1	2.29	0.48
4:H:33:MET:HE1	4:H:60:SER:N	2.28	0.48
4:H:128:CYS:O	4:H:161:GLN:HG3	2.14	0.48
1:E:26:GLY:HA3	1:E:34:VAL:CG1	2.44	0.47
2:F:16:GLU:HA	6:F:203:HOH:O	2.13	0.47
2:B:47:GLU:HG3	2:B:48:LYS:H	1.79	0.47
4:H:170:THR:OG1	4:H:171:HIS:N	2.44	0.47
1:E:79:ARG:HB3	4:H:44:MET:CE	2.44	0.47
2:F:51:HIS:HB3	2:F:66:TYR:CD2	2.49	0.47
1:A:249:VAL:HG22	1:A:257:TYR:CZ	2.49	0.47
4:H:72:ASP:OD1	4:H:72:ASP:N	2.48	0.47
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.49	0.47
2:F:6:LYS:O	2:F:27:VAL:HA	2.15	0.46
1:A:201:LEU:HD21	1:A:254:GLU:HG3	1.96	0.46
1:E:51:TRP:CZ2	1:E:179:LEU:HD11	2.50	0.46
4:D:24:VAL:HG12	4:D:66:ILE:HB	1.97	0.46
1:E:258:THR:HG23	1:E:271:THR:HG23	1.97	0.46
4:D:10:LEU:HG	4:D:97:LEU:CD2	2.44	0.46
1:E:219:ARG:NH2	1:E:256:ARG:HH12	2.14	0.46
1:E:254:GLU:OE1	1:E:254:GLU:N	2.38	0.46
4:D:54:GLU:O	4:D:55:HIS:HB2	2.16	0.46
1:A:141:GLN:O	1:A:145:ARG:HG3	2.16	0.45
4:D:102:ILE:HG22	4:D:188:TRP:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:LEU:HG	1:A:168:LEU:HD23	1.98	0.45
2:B:47:GLU:HG3	2:B:48:LYS:N	2.31	0.45
1:E:26:GLY:HA3	1:E:34:VAL:HG12	1.99	0.45
1:E:262[B]:GLN:OE1	1:E:269:PRO:HG3	2.16	0.45
1:A:73:THR:HG23	3:C:8:VAL:HG22	1.97	0.45
1:E:214:THR:HB	1:E:262[B]:GLN:HB3	1.98	0.45
3:G:1:ILE:HD13	3:G:1:ILE:HA	1.83	0.45
4:H:145:ALA:N	5:H:301:SO4:O3	2.40	0.45
1:E:28:VAL:HG23	1:E:33:PHE:CD1	2.51	0.44
1:E:103:LEU:HG	1:E:168:LEU:HD23	1.99	0.44
4:D:11:LEU:HD23	4:D:13:HIS:NE2	2.32	0.44
4:D:26:LEU:HD12	4:D:26:LEU:N	2.32	0.44
4:H:9:SER:O	4:H:28:CYS:HA	2.17	0.44
1:A:167:TRP:CE2	3:C:1:ILE:HG13	2.53	0.44
2:B:23:LEU:O	2:B:67:TYR:HA	2.17	0.44
1:A:26:GLY:HA3	1:A:34:VAL:HG12	2.00	0.44
1:E:230:LEU:HD21	1:E:245:ALA:HB2	1.98	0.44
2:F:29:GLY:HA2	2:F:61:SER:HB3	2.00	0.44
1:A:13:SER:HB3	1:A:78:LEU:HD13	1.99	0.44
1:E:117:ALA:HB2	2:F:60:TRP:CE2	2.52	0.44
4:D:72:ASP:OD1	4:D:72:ASP:N	2.51	0.44
4:H:118:VAL:HG21	4:H:169:ALA:HB2	2.00	0.44
4:H:149:ARG:NH2	5:H:302:SO4:O3	2.51	0.44
2:B:24:ASN:HB3	2:B:65:LEU:HD11	2.00	0.43
1:E:58:GLU:H	1:E:58:GLU:CD	2.24	0.43
4:H:35:GLU:O	4:H:36:HIS:ND1	2.47	0.43
4:H:7:LYS:HG3	4:H:94:SER:HA	2.00	0.43
1:E:63:GLU:OE2	3:G:1:ILE:HD12	2.18	0.43
1:A:68:LYS:O	1:A:72:GLN:HG3	2.19	0.43
2:B:51:HIS:HB3	2:B:66:TYR:CD2	2.54	0.43
4:H:26:LEU:HD12	4:H:26:LEU:N	2.34	0.43
4:H:41:ARG:HD3	4:H:77:TYR:CZ	2.54	0.42
4:H:129:SER:OG	4:H:159:THR:HG21	2.19	0.42
1:A:35:GLN:HG3	2:B:53:ASP:OD2	2.18	0.42
1:A:254:GLU:OE1	1:A:254:GLU:N	2.42	0.42
1:E:126:LEU:HD12	1:E:132:SER:O	2.19	0.42
4:H:119:LEU:HD12	4:H:200:THR:C	2.45	0.42
4:H:6:ARG:HA	4:H:6:ARG:HD2	1.85	0.42
1:A:63:GLU:OE2	1:A:66:LYS:NZ	2.46	0.42
1:A:224:GLN:O	1:A:228:THR:CG2	2.67	0.42
1:A:201:LEU:HD23	1:A:249:VAL:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1:ILE:HD13	3:C:1:ILE:HA	1.91	0.42
1:E:51:TRP:CE2	1:E:179:LEU:HD11	2.54	0.42
4:D:61:LYS:O	4:D:61:LYS:HG3	2.20	0.42
4:H:128:CYS:O	4:H:161:GLN:HA	2.19	0.42
1:E:34:VAL:HG22	1:E:35:GLN:N	2.35	0.41
4:H:6:ARG:O	4:H:91:SER:HB2	2.20	0.41
4:H:59:VAL:HG12	4:H:61:LYS:HG3	2.02	0.41
1:E:220:ASP:OD2	1:E:256:ARG:NH2	2.51	0.41
1:E:266:LEU:HD13	1:E:270:LEU:HG	2.02	0.41
1:A:203:CYS:O	1:A:244:TRP:HA	2.20	0.41
2:F:79:ALA:HB2	2:F:94:LYS:HD3	2.01	0.41
4:H:86:SER:HA	4:H:87:PRO:C	2.46	0.41
1:A:184:HIS:HB3	1:A:265:GLY:O	2.21	0.41
4:H:25:ILE:HD12	4:H:25:ILE:N	2.35	0.41
1:E:49:ALA:O	1:E:53:GLU:HG3	2.21	0.41
1:E:0:MET:HB2	1:E:105:PRO:HB2	2.02	0.41
1:E:27:TYR:CE2	1:E:32:GLN:HB2	2.55	0.41
1:E:14:ARG:HB3	1:E:17:ARG:HB2	2.03	0.41
1:A:234:ARG:HD2	2:B:10:TYR:CE1	2.55	0.41
4:D:113:GLN:O	4:D:124:VAL:HA	2.19	0.41
4:H:100:VAL:HG11	4:H:188:TRP:CE2	2.56	0.41
2:F:51:HIS:HA	2:F:65:LEU:O	2.21	0.41
1:E:1:MET:HG2	1:E:264:GLU:CD	2.46	0.40
4:D:118:VAL:HG21	4:D:169:ALA:CB	2.51	0.40
2:F:23:LEU:O	2:F:67:TYR:HA	2.20	0.40
4:D:113:GLN:HA	4:D:113:GLN:OE1	2.22	0.40
4:H:16:ARG:HH12	4:H:147:GLU:HG2	1.85	0.40
1:E:35:GLN:NE2	1:E:37:ASP:HB2	2.36	0.40
1:A:63:GLU:OE2	3:C:1:ILE:HD12	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	273/279 (98%)	267 (98%)	6 (2%)	0	100	100
1	E	274/279 (98%)	265 (97%)	9 (3%)	0	100	100
2	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
2	F	98/100 (98%)	97 (99%)	1 (1%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
3	G	7/9 (78%)	7 (100%)	0	0	100	100
4	D	177/204 (87%)	169 (96%)	8 (4%)	0	100	100
4	H	193/204 (95%)	184 (95%)	9 (5%)	0	100	100
All	All	1127/1184 (95%)	1092 (97%)	35 (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	222/234 (95%)	220 (99%)	2 (1%)	70	83
1	E	228/234 (97%)	228 (100%)	0	100	100
2	B	92/95 (97%)	92 (100%)	0	100	100
2	F	92/95 (97%)	90 (98%)	2 (2%)	45	69
3	C	7/7 (100%)	7 (100%)	0	100	100
3	G	7/7 (100%)	7 (100%)	0	100	100
4	D	145/176 (82%)	141 (97%)	4 (3%)	38	62
4	H	166/176 (94%)	165 (99%)	1 (1%)	78	89
All	All	959/1024 (94%)	950 (99%)	9 (1%)	70	83

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	LYS
1	A	216	THR

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Mol	Chain	Res	Type
2	F	48	LYS
2	F	70	PHE
4	D	61	LYS
4	D	68	ARG
4	D	147	GLU
4	D	182	ARG
4	H	147	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	188	HIS
2	B	51	HIS
2	F	13	HIS
4	D	123	ASN
4	H	27	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

17 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	$\#\|Z\| > 2$
5	SO4	D	303	-	4,4,4	0.63	0	6,6,6	0.18	0
5	SO4	E	301	-	4,4,4	0.80	0	6,6,6	0.25	0
5	SO4	D	302	-	4,4,4	0.65	0	6,6,6	0.11	0
5	SO4	A	302	-	4,4,4	0.82	0	6,6,6	0.11	0
5	SO4	H	303	-	4,4,4	0.65	0	6,6,6	0.10	0
5	SO4	F	103	-	4,4,4	0.68	0	6,6,6	0.16	0
5	SO4	A	303	-	4,4,4	0.70	0	6,6,6	0.11	0
5	SO4	E	303	-	4,4,4	0.69	0	6,6,6	0.18	0
5	SO4	B	102	-	4,4,4	0.71	0	6,6,6	0.15	0
5	SO4	F	102	-	4,4,4	0.65	0	6,6,6	0.11	0
5	SO4	A	301	-	4,4,4	0.69	0	6,6,6	0.14	0
5	SO4	E	302	-	4,4,4	0.71	0	6,6,6	0.12	0
5	SO4	D	301	-	4,4,4	0.61	0	6,6,6	0.11	0
5	SO4	F	101	-	4,4,4	0.69	0	6,6,6	0.19	0
5	SO4	H	302	-	4,4,4	0.66	0	6,6,6	0.11	0
5	SO4	B	101	-	4,4,4	0.69	0	6,6,6	0.12	0
5	SO4	H	301	-	4,4,4	0.63	0	6,6,6	0.15	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	H	302	SO4	1	0
5	H	301	SO4	1	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

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	275/279 (98%)	-0.01	2 (0%) 84 80	31, 47, 73, 103	0
1	E	275/279 (98%)	-0.08	1 (0%) 88 86	27, 46, 78, 98	1 (0%)
2	B	100/100 (100%)	-0.01	1 (1%) 79 74	31, 48, 77, 86	0
2	F	100/100 (100%)	0.09	2 (2%) 65 57	31, 47, 73, 85	0
3	C	9/9 (100%)	-0.16	0 100 100	42, 44, 53, 55	0
3	G	9/9 (100%)	0.18	0 100 100	38, 44, 50, 57	0
4	D	183/204 (89%)	0.50	13 (7%) 22 19	36, 56, 119, 161	0
4	H	195/204 (95%)	0.22	2 (1%) 79 74	33, 52, 88, 111	0
All	All	1146/1184 (96%)	0.10	21 (1%) 67 59	27, 49, 89, 161	1 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	41	ALA	3.7
1	A	90	ALA	3.5
4	D	64	PHE	3.3
4	D	28	CYS	3.0
2	B	99	MET	3.0
4	D	56	HIS	2.8
4	D	33	MET	2.8
4	D	6	ARG	2.7
4	D	32	VAL	2.5
4	D	35	GLU	2.4
2	F	34	ASP	2.4
4	D	156	VAL	2.4
4	D	36	HIS	2.2
4	H	57	ASP	2.2
2	F	0	MET	2.2
4	D	34	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
4	H	29	TRP	2.1
4	D	62	ALA	2.1
4	D	59	VAL	2.1
4	D	55	HIS	2.1
1	E	197	HIS	2.1

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 oligosaccharides 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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	D	301	5/5	0.55	0.17	97,111,127,136	0
5	SO4	A	303	5/5	0.75	0.16	80,83,119,121	0
5	SO4	F	103	5/5	0.76	0.27	89,90,106,130	0
5	SO4	F	102	5/5	0.77	0.15	75,91,126,132	0
5	SO4	B	102	5/5	0.80	0.26	70,86,91,116	0
5	SO4	E	302	5/5	0.83	0.24	79,80,118,119	0
5	SO4	E	303	5/5	0.84	0.35	74,83,95,118	0
5	SO4	F	101	5/5	0.85	0.28	77,78,109,117	0
5	SO4	A	302	5/5	0.85	0.18	51,55,68,100	0
5	SO4	D	303	5/5	0.85	0.24	76,81,91,104	0
5	SO4	A	301	5/5	0.86	0.17	65,68,110,114	0
5	SO4	B	101	5/5	0.86	0.23	69,80,82,109	0
5	SO4	H	303	5/5	0.87	0.17	75,83,88,103	0
5	SO4	D	302	5/5	0.88	0.16	65,74,83,85	0
5	SO4	H	302	5/5	0.89	0.11	57,65,84,84	0
5	SO4	E	301	5/5	0.91	0.17	46,55,68,96	0
5	SO4	H	301	5/5	0.98	0.05	46,51,56,60	0

6.5 Other polymers (i)

There are no such residues in this entry.