



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:02 AM UTC

PDB ID : 2OJE / pdb_00002oje
Title : Mycoplasma arthritidis-derived mitogen complexed with class II MHC molecule HLA-DR1/HA complex in the presence of EDTA
Authors : Li, H.; Zhao, Y.; Guo, Y.; Li, Z.; Eisele, L.; Mourad, W.
Deposited on : 2007-01-12
Resolution : 3.00 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:

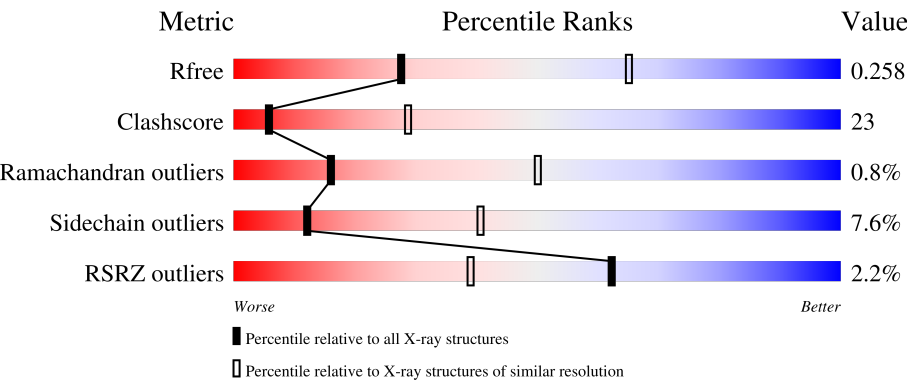
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	180	2% 60% 34% 6%
1	E	180	% 61% 36% •
2	B	190	4% 56% 39% 5% •
2	F	190	4% 53% 42% 5%
3	C	13	38% 54% 8%

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Mol	Chain	Length	Quality of chain
3	G	13	8% 54% 38% 8%
4	D	214	2% 57% 36% 7%
4	H	214	% 54% 42% •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10010 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 HLA class II histocompatibility antigen, DR alpha chain precursor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	Se	0	0	0
			1483	960	241	277	2	3			
1	E	180	Total	C	N	O	S	Se	0	0	0
			1483	960	241	277	2	3			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MSE	MET	modified residue	UNP P01903
A	36	MSE	MET	modified residue	UNP P01903
A	73	MSE	MET	modified residue	UNP P01903
E	23	MSE	MET	modified residue	UNP P01903
E	36	MSE	MET	modified residue	UNP P01903
E	73	MSE	MET	modified residue	UNP P01903

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DRB1-1 beta chain precursor.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	190	Total	C	N	O	S		0	0	0
			1557	979	279	293	6				
2	F	190	Total	C	N	O	S		0	0	0
			1557	979	279	293	6				

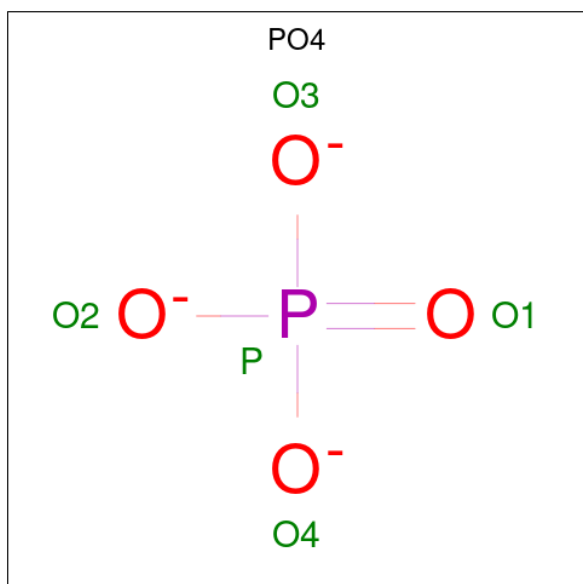
- Molecule 3 is a protein called haemagglutinin peptide 306-318.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	13	Total	C	N	O	0	0	0
			106	69	18	19			
3	G	13	Total	C	N	O	0	0	0
			102	66	17	19			

- Molecule 4 is a protein called Superantigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	214	Total	C	N	O	S	0	0	0
			1792	1157	302	328	5			
4	H	214	Total	C	N	O	S	0	0	0
			1792	1157	302	328	5			

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	25	Total	O	0	0
			25	25		
6	B	23	Total	O	0	0
			23	23		
6	C	1	Total	O	0	0
			1	1		

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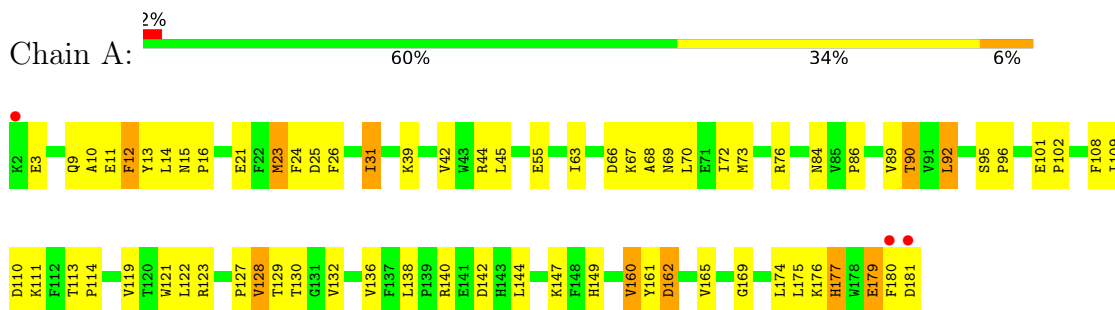
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	19	Total 19	O 19	0	0
6	E	34	Total 34	O 34	0	0
6	F	4	Total 4	O 4	0	0
6	H	12	Total 12	O 12	0	0

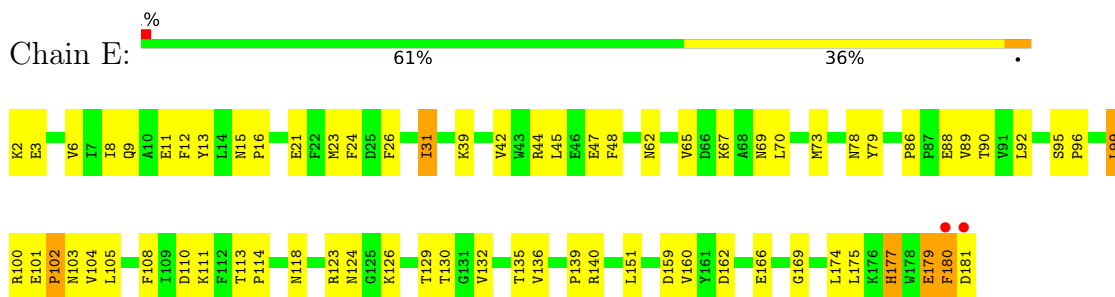
3 Residue-property plots [i](#)

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.

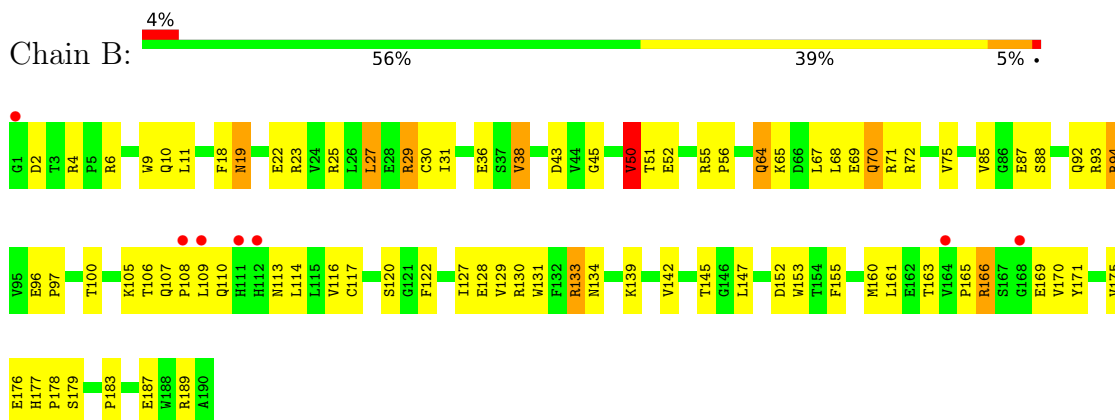
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain precursor



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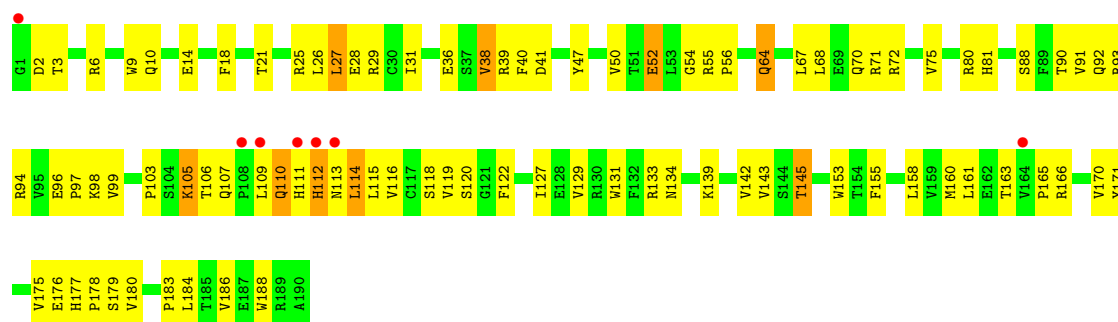


- Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain precursor

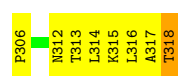


- Molecule 2: HLA class II histocompatibility antigen, DRB1-1 beta chain precursor

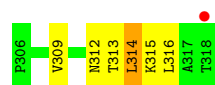




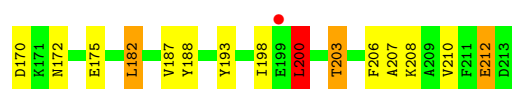
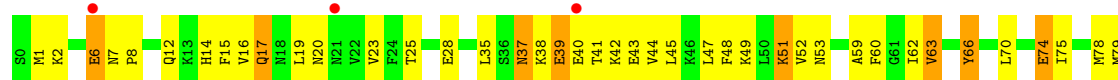
• Molecule 3: haemagglutinin peptide 306-318



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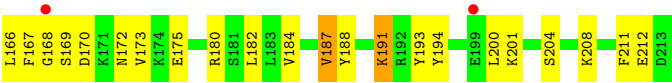


• Molecule 4: Superantigen



• Molecule 4: Superantigen





4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	137.74Å 179.56Å 179.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.22 – 3.00 40.22 – 3.00	Depositor EDS
% Data completeness (in resolution range)	89.8 (40.22-3.00) 89.7 (40.22-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	12.40	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.70 (at 3.01Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.211 , 0.261 0.209 , 0.258	Depositor DCC
R_{free} test set	2850 reflections (7.01%)	wwPDB-VP
Wilson B-factor (Å ²)	45.7	Xtriage
Anisotropy	0.454	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.046 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10010	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

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: 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	0.51	0/1525	0.96	1/2072 (0.0%)
1	E	0.48	0/1525	0.95	1/2072 (0.0%)
2	B	0.49	0/1597	0.94	3/2168 (0.1%)
2	F	0.45	0/1597	0.92	3/2168 (0.1%)
3	C	0.44	0/107	1.00	0/141
3	G	0.56	0/103	1.00	0/137
4	D	0.46	0/1822	0.93	6/2439 (0.2%)
4	H	0.46	0/1822	0.95	8/2439 (0.3%)
All	All	0.47	0/10098	0.94	22/13636 (0.2%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	175	GLU	N-CA-C	8.82	120.66	111.14
4	D	175	GLU	N-CA-C	8.42	120.54	111.36
2	F	50	VAL	N-CA-C	-8.18	105.27	111.90
2	B	120	SER	N-CA-C	7.05	119.88	109.24
2	B	50	VAL	N-CA-C	-6.83	106.13	112.96
1	A	31	ILE	N-CA-C	-6.66	105.26	111.45
2	F	120	SER	N-CA-C	6.58	119.17	109.24
2	F	145	THR	N-CA-C	-6.48	105.38	113.28
2	B	145	THR	N-CA-C	-5.91	106.03	113.18
1	E	31	ILE	N-CA-C	-5.63	106.21	111.45
4	D	20	ASN	N-CA-C	5.57	120.97	113.72
4	H	20	ASN	N-CA-C	5.57	120.96	113.72
4	D	66	TYR	N-CA-C	5.44	119.54	111.87
4	H	147	LYS	N-CA-C	5.44	117.64	111.11
4	D	23	VAL	N-CA-C	5.42	116.00	108.84
4	H	66	TYR	N-CA-C	5.32	119.36	111.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^o)	Ideal(^o)
4	H	6	GLU	N-CA-C	5.26	117.43	111.11
4	H	23	VAL	N-CA-C	5.22	115.83	109.30
4	D	7	ASN	CA-C-N	5.18	125.10	119.76
4	D	7	ASN	C-N-CA	5.18	125.10	119.76
4	H	7	ASN	CA-C-N	5.13	125.05	119.76
4	H	7	ASN	C-N-CA	5.13	125.05	119.76

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	1483	0	1420	77	0
1	E	1483	0	1420	62	1
2	B	1557	0	1488	90	0
2	F	1557	0	1488	85	0
3	C	106	0	119	13	0
3	G	102	0	108	10	0
4	D	1792	0	1836	83	0
4	H	1792	0	1836	75	0
5	C	5	0	0	0	0
5	D	5	0	0	0	0
5	E	5	0	0	0	0
5	H	5	0	0	0	0
6	A	25	0	0	0	0
6	B	23	0	0	0	0
6	C	1	0	0	0	0
6	D	19	0	0	1	0
6	E	34	0	0	0	0
6	F	4	0	0	0	0
6	H	12	0	0	0	0
All	All	10010	0	9715	452	1

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 23.

All (452) 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:B:166:ARG:HB2	2:B:166:ARG:HH21	1.24	1.02
2:F:107:GLN:HE21	2:F:109:LEU:HD21	1.22	1.01
4:H:1:MET:CE	4:H:132:TRP:HB3	1.96	0.95
4:H:1:MET:HE1	4:H:132:TRP:HB3	1.51	0.91
4:H:160:ILE:H	4:H:160:ILE:HD12	1.33	0.91
4:D:45:LEU:HD11	4:D:49:LYS:HE3	1.51	0.90
4:H:51:LYS:HG3	4:H:104:ILE:HG23	1.53	0.88
2:B:166:ARG:HB2	2:B:166:ARG:NH2	1.88	0.88
2:F:107:GLN:NE2	2:F:109:LEU:HD21	1.88	0.87
4:D:16:VAL:HG21	4:D:81:LEU:HD11	1.55	0.86
1:A:16:PRO:HD2	2:B:6:ARG:HD2	1.56	0.85
2:B:105:LYS:HD2	2:B:110:GLN:O	1.76	0.85
1:A:90:THR:HG23	1:A:108:PHE:HB2	1.59	0.83
4:D:2:LYS:HE2	4:D:2:LYS:N	1.92	0.83
2:B:106:THR:HG23	2:B:107:GLN:HG3	1.61	0.83
1:A:10:ALA:HB3	1:A:23:MSE:HE1	1.59	0.82
4:D:144:ILE:HD13	4:H:46:LYS:HD3	1.62	0.81
2:F:134:ASN:HD21	2:F:170:VAL:H	1.30	0.80
4:D:51:LYS:HG3	4:D:104:ILE:HG23	1.62	0.80
1:A:179:GLU:O	1:A:181:ASP:N	2.14	0.80
1:E:39:LYS:HE2	1:E:39:LYS:O	1.81	0.80
2:F:105:LYS:HE3	2:F:112:HIS:HA	1.63	0.79
2:F:2:ASP:CG	2:F:6:ARG:HH12	1.92	0.78
1:A:95:SER:HB2	1:A:96:PRO:HD2	1.67	0.77
2:F:106:THR:HG23	2:F:107:GLN:HG3	1.66	0.76
2:F:113:ASN:HB3	2:F:114:LEU:HD23	1.68	0.76
2:B:68:LEU:O	2:B:72:ARG:HG3	1.85	0.76
4:D:37:ASN:HD22	4:D:38:LYS:N	1.82	0.76
1:A:70:LEU:HD23	2:B:9:TRP:HB2	1.66	0.75
2:B:25:ARG:HD2	2:B:43:ASP:OD1	1.87	0.75
2:F:96:GLU:HA	2:F:179:SER:OG	1.87	0.75
4:D:59:ALA:HA	4:D:79:MET:HE1	1.67	0.74
1:A:10:ALA:HB3	1:A:23:MSE:CE	2.17	0.74
2:F:107:GLN:HE21	2:F:109:LEU:CD2	1.97	0.74
4:D:1:MET:C	4:D:2:LYS:HE2	2.11	0.74
2:B:133:ARG:HG3	2:B:171:TYR:CE1	2.23	0.74
1:A:179:GLU:C	1:A:181:ASP:H	1.96	0.73
2:B:108:PRO:HG2	2:B:109:LEU:HD12	1.71	0.72
1:E:123:ARG:O	1:E:126:LYS:HG2	1.90	0.72
2:B:25:ARG:HH21	2:B:27:LEU:HD21	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:200:LEU:HB2	6:D:229:HOH:O	1.90	0.72
4:H:16:VAL:HG21	4:H:81:LEU:HD11	1.70	0.72
2:F:64:GLN:HG2	4:H:15:PHE:CE2	2.25	0.72
1:E:23:MSE:HE1	1:E:139:PRO:HD3	1.71	0.72
1:A:23:MSE:HE3	1:A:23:MSE:O	1.90	0.71
4:H:208:LYS:O	4:H:212:GLU:HB2	1.90	0.71
4:H:170:ASP:HB3	4:H:173:VAL:HG23	1.73	0.70
2:F:93:ARG:O	2:F:94:ARG:HD3	1.91	0.70
2:F:55:ARG:HB2	2:F:56:PRO:HD3	1.72	0.70
1:E:124:ASN:ND2	1:E:160:VAL:H	1.89	0.70
1:E:21:GLU:OE2	1:E:136:VAL:HG22	1.90	0.70
4:D:126:LYS:HD2	4:D:126:LYS:C	2.17	0.69
4:H:164:ARG:HG3	4:H:164:ARG:HH11	1.56	0.69
1:E:129:THR:O	1:E:132:VAL:HG22	1.93	0.69
4:H:45:LEU:HD11	4:H:49:LYS:HE3	1.73	0.69
4:H:160:ILE:HD12	4:H:160:ILE:N	2.07	0.69
2:B:87:GLU:O	2:B:92:GLN:HG2	1.92	0.69
1:A:39:LYS:O	1:A:39:LYS:HD3	1.92	0.69
2:B:94:ARG:HH11	2:B:94:ARG:HG2	1.57	0.69
2:F:110:GLN:HE21	2:F:111:HIS:H	1.40	0.69
1:A:44:ARG:O	1:A:45:LEU:HD23	1.93	0.68
2:F:176:GLU:HG2	2:F:183:PRO:HB3	1.75	0.68
2:B:64:GLN:HE21	2:B:64:GLN:N	1.92	0.68
4:D:1:MET:HE2	4:D:129:GLN:HG2	1.76	0.68
2:B:19:ASN:HB3	2:B:22:GLU:OE2	1.92	0.68
2:F:134:ASN:ND2	2:F:170:VAL:H	1.92	0.68
4:H:45:LEU:CD1	4:H:49:LYS:HE3	2.23	0.67
4:H:98:GLU:HG3	4:H:99:GLN:N	2.09	0.67
1:A:92:LEU:HD23	1:A:92:LEU:N	2.10	0.67
4:D:35:LEU:HB3	4:D:94:ALA:CB	2.24	0.67
4:H:154:ARG:CZ	4:H:154:ARG:HB2	2.24	0.67
4:H:1:MET:HE2	4:H:132:TRP:HB3	1.76	0.67
1:E:99:LEU:HD12	1:E:100:ARG:HG2	1.77	0.67
2:F:106:THR:CG2	2:F:110:GLN:HG3	2.25	0.67
4:H:108:ASP:HA	4:H:111:MET:HE3	1.75	0.66
2:F:103:PRO:HD3	2:F:188:TRP:CH2	2.31	0.66
4:H:1:MET:HE1	4:H:132:TRP:CB	2.23	0.66
4:H:96:ASN:OD1	4:H:98:GLU:HG2	1.94	0.66
2:B:114:LEU:HD23	2:B:114:LEU:H	1.61	0.66
1:E:13:TYR:CE2	1:E:67:LYS:HG3	2.31	0.66
2:F:114:LEU:HD23	2:F:114:LEU:H	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:44:ARG:HE	1:E:135:THR:HG22	1.59	0.65
4:H:160:ILE:H	4:H:160:ILE:CD1	2.07	0.65
2:B:85:VAL:HG13	3:C:306:PRO:HB2	1.77	0.65
1:E:3:GLU:OE1	1:E:6:VAL:HG22	1.96	0.65
2:F:180:VAL:HG11	2:F:184:LEU:HD13	1.79	0.65
4:D:1:MET:CE	4:D:129:GLN:HG2	2.27	0.65
3:G:315:LYS:HD3	3:G:316:LEU:O	1.96	0.65
3:C:315:LYS:HZ2	4:D:19:LEU:HD23	1.62	0.65
1:E:124:ASN:HD21	1:E:160:VAL:H	1.44	0.65
1:E:70:LEU:HD13	2:F:9:TRP:HB2	1.78	0.65
1:A:14:LEU:HD11	2:B:6:ARG:HB3	1.77	0.64
1:A:111:LYS:HG2	1:A:140:ARG:CZ	2.25	0.64
4:D:37:ASN:HD22	4:D:38:LYS:H	1.45	0.64
2:B:134:ASN:HD21	2:B:170:VAL:H	1.46	0.64
4:D:107:LEU:O	4:D:111:MET:HG3	1.97	0.64
1:E:99:LEU:CD1	1:E:100:ARG:HG2	2.28	0.64
2:F:180:VAL:HG21	2:F:184:LEU:HD11	1.79	0.64
1:A:23:MSE:HG2	1:A:24:PHE:N	2.13	0.63
4:D:98:GLU:O	4:D:102:ARG:HG3	1.98	0.63
2:F:180:VAL:HG11	2:F:184:LEU:CD1	2.28	0.63
2:B:45:GLY:O	2:B:72:ARG:NH2	2.31	0.63
1:A:16:PRO:HD2	2:B:6:ARG:CD	2.29	0.62
1:A:179:GLU:O	1:A:179:GLU:HG2	1.99	0.62
2:B:25:ARG:NH2	2:B:27:LEU:HD21	2.14	0.62
2:B:166:ARG:HH21	2:B:166:ARG:CB	2.07	0.62
2:B:128:GLU:OE1	2:B:130:ARG:NH1	2.32	0.62
1:E:123:ARG:HD2	1:E:126:LYS:HE3	1.81	0.62
2:F:105:LYS:HG3	2:F:111:HIS:O	2.00	0.62
4:D:113:LYS:HE3	4:D:117:ASP:OD1	2.00	0.62
4:H:143:LYS:O	4:H:194:TYR:OH	2.17	0.61
4:D:16:VAL:HG21	4:D:81:LEU:CD1	2.28	0.61
2:B:19:ASN:HB3	2:B:22:GLU:CD	2.25	0.61
4:H:113:LYS:NZ	4:H:117:ASP:OD1	2.33	0.61
2:B:114:LEU:HD12	2:B:160:MET:HB3	1.82	0.61
4:H:143:LYS:HE3	4:H:193:TYR:CE2	2.36	0.60
3:C:312:ASN:HB2	4:D:14:HIS:CE1	2.37	0.60
4:D:208:LYS:O	4:D:212:GLU:HB2	2.02	0.60
1:E:179:GLU:O	1:E:181:ASP:N	2.35	0.60
2:B:64:GLN:HG2	4:D:15:PHE:CE2	2.36	0.60
4:D:105:ALA:O	4:D:109:GLU:HG3	2.02	0.60
4:H:65:ASP:OD2	4:H:204:SER:HB2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:39:GLU:HG2	4:H:42:LYS:HE3	1.84	0.60
1:E:111:LYS:HG2	1:E:140:ARG:CZ	2.31	0.60
4:H:59:ALA:HA	4:H:79:MET:HE1	1.84	0.60
4:H:180:ARG:O	4:H:184:VAL:HG23	2.02	0.60
2:F:114:LEU:HD23	2:F:114:LEU:N	2.16	0.59
4:D:1:MET:HE3	4:D:122:ILE:CG2	2.31	0.59
2:F:134:ASN:ND2	2:F:170:VAL:HG12	2.18	0.59
2:F:106:THR:HG22	2:F:110:GLN:HG3	1.84	0.59
2:F:145:THR:HG23	2:F:158:LEU:HB2	1.85	0.59
2:B:106:THR:CG2	2:B:110:GLN:HG3	2.32	0.59
2:F:114:LEU:HD12	2:F:160:MET:HG2	1.85	0.59
4:H:41:THR:HG21	4:H:95:ASN:HD22	1.67	0.59
4:H:105:ALA:O	4:H:109:GLU:HG3	2.01	0.58
1:A:179:GLU:C	1:A:181:ASP:N	2.61	0.58
2:B:163:THR:O	2:B:165:PRO:HD3	2.03	0.58
1:A:113:THR:OG1	1:A:114:PRO:HA	2.02	0.58
1:E:73:MSE:HG2	3:G:316:LEU:CD1	2.33	0.58
4:H:164:ARG:HG3	4:H:164:ARG:NH1	2.17	0.58
2:B:65:LYS:O	2:B:69:GLU:HG3	2.03	0.58
4:D:6:GLU:CD	4:D:6:GLU:H	2.09	0.58
2:F:161:LEU:HG	2:F:163:THR:HG23	1.85	0.58
2:F:52:GLU:OE1	2:F:55:ARG:NH2	2.37	0.58
1:A:160:VAL:HG23	1:A:179:GLU:HB3	1.86	0.58
1:E:16:PRO:HD2	2:F:6:ARG:HD3	1.85	0.58
1:A:12:PHE:CD1	1:A:12:PHE:C	2.82	0.58
2:B:96:GLU:HA	2:B:179:SER:OG	2.03	0.58
2:B:176:GLU:HG2	2:B:183:PRO:HB3	1.86	0.58
4:D:60:PHE:HA	4:D:63:VAL:HG12	1.85	0.58
1:A:110:ASP:OD1	1:A:111:LYS:N	2.37	0.57
4:H:25:THR:OG1	4:H:28:GLU:HG3	2.04	0.57
4:D:182:LEU:HG	4:D:206:PHE:CE1	2.39	0.57
4:H:146:LEU:CD2	4:H:162:LYS:HE2	2.34	0.57
1:A:162:ASP:N	1:A:162:ASP:OD2	2.38	0.57
4:D:14:HIS:HD2	4:D:78:MET:SD	2.28	0.57
1:E:180:PHE:CD2	1:E:181:ASP:N	2.73	0.57
1:A:3:GLU:HB2	2:B:18:PHE:CE2	2.40	0.56
1:E:113:THR:OG1	1:E:114:PRO:HA	2.05	0.56
2:B:30:CYS:HB2	2:B:38:VAL:HG23	1.87	0.56
2:B:134:ASN:ND2	2:B:170:VAL:H	2.02	0.56
2:F:99:VAL:HG21	2:F:175:VAL:HG21	1.86	0.56
2:B:25:ARG:HE	2:B:27:LEU:HD23	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:35:LEU:HB3	4:D:94:ALA:HB2	1.87	0.56
2:F:52:GLU:OE1	2:F:52:GLU:HA	2.05	0.56
4:D:203:THR:HG22	4:D:207:ALA:CB	2.36	0.56
4:H:17:GLN:H	4:H:17:GLN:NE2	2.03	0.56
4:D:96:ASN:O	4:D:100:ILE:HD12	2.06	0.56
2:F:127:ILE:HD11	2:F:175:VAL:HG13	1.87	0.56
4:D:85:VAL:O	4:D:88:ASP:HB2	2.06	0.56
2:F:127:ILE:HD11	2:F:175:VAL:CG1	2.36	0.56
2:F:67:LEU:HD21	3:G:314:LEU:HD21	1.88	0.55
2:B:127:ILE:HD11	2:B:175:VAL:CG1	2.36	0.55
4:H:41:THR:CG2	4:H:95:ASN:HD22	2.19	0.55
1:E:15:ASN:ND2	1:E:70:LEU:HD23	2.21	0.55
1:E:45:LEU:HD12	1:E:48:PHE:CZ	2.42	0.55
1:E:162:ASP:CG	1:E:175:LEU:HD21	2.32	0.55
1:E:12:PHE:CD1	1:E:12:PHE:C	2.84	0.55
4:H:156:GLY:HA2	4:H:188:TYR:OH	2.06	0.55
4:H:170:ASP:HB3	4:H:173:VAL:CG2	2.35	0.55
1:E:162:ASP:HB3	1:E:177:HIS:HA	1.89	0.55
2:B:55:ARG:HB2	2:B:56:PRO:HD3	1.88	0.54
1:A:3:GLU:HA	2:B:18:PHE:CD2	2.42	0.54
3:C:312:ASN:HB2	4:D:14:HIS:ND1	2.22	0.54
1:E:110:ASP:OD2	1:E:111:LYS:N	2.37	0.54
2:B:11:LEU:HD22	3:C:313:THR:HG23	1.89	0.54
2:B:85:VAL:HG13	3:C:306:PRO:CB	2.37	0.54
2:B:166:ARG:HG3	2:B:169:GLU:CD	2.33	0.54
1:A:73:MSE:HG2	3:C:316:LEU:HD11	1.90	0.54
4:D:66:TYR:CD2	4:D:118:LEU:HD21	2.43	0.54
4:H:138:LEU:HD13	4:H:167:PHE:CD2	2.43	0.54
2:B:50:VAL:HG23	2:B:51:THR:HG23	1.89	0.54
2:F:94:ARG:HG3	2:F:94:ARG:HH11	1.73	0.54
2:F:176:GLU:CG	2:F:183:PRO:HB3	2.37	0.54
4:D:15:PHE:HA	4:D:17:GLN:HE22	1.73	0.54
1:A:174:LEU:HD21	1:A:176:LYS:HD3	1.90	0.53
2:F:131:TRP:CD1	2:F:161:LEU:HB2	2.43	0.53
1:A:121:TRP:HB3	1:A:128:VAL:HG22	1.90	0.53
1:A:147:LYS:HE3	1:A:149:HIS:HE1	1.73	0.53
2:B:139:LYS:O	2:B:142:VAL:HG22	2.08	0.53
1:E:160:VAL:HG21	1:E:177:HIS:CE1	2.42	0.53
4:D:16:VAL:O	4:D:16:VAL:HG22	2.08	0.53
2:F:40:PHE:HB2	2:F:47:TYR:CE1	2.44	0.53
2:F:105:LYS:CE	2:F:112:HIS:HA	2.35	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:VAL:HG13	1:E:160:VAL:O	2.08	0.53
1:A:70:LEU:HD23	2:B:9:TRP:CB	2.38	0.53
4:D:1:MET:HE3	4:D:122:ILE:HG21	1.90	0.53
2:B:97:PRO:HB3	2:B:122:PHE:HB3	1.91	0.53
4:D:102:ARG:O	4:D:106:ILE:HG13	2.09	0.53
4:H:6:GLU:O	4:H:8:PRO:HD3	2.09	0.53
1:A:136:VAL:O	1:A:138:LEU:HD12	2.09	0.52
1:A:89:VAL:HG21	1:A:165:VAL:HG21	1.91	0.52
4:D:6:GLU:O	4:D:8:PRO:HD3	2.10	0.52
4:D:60:PHE:HA	4:D:63:VAL:CG1	2.39	0.52
1:E:129:THR:O	1:E:130:THR:C	2.52	0.52
4:D:45:LEU:CD1	4:D:49:LYS:HE3	2.32	0.52
4:D:140:LYS:O	4:D:143:LYS:HB3	2.09	0.52
1:A:13:TYR:CE2	1:A:67:LYS:HG3	2.44	0.52
4:D:75:ILE:CD1	4:D:118:LEU:HA	2.40	0.52
2:F:122:PHE:CE1	2:F:155:PHE:HB2	2.45	0.52
4:H:6:GLU:HA	4:H:6:GLU:OE1	2.09	0.52
4:H:140:LYS:O	4:H:143:LYS:HB3	2.10	0.52
2:B:18:PHE:HD1	2:B:23:ARG:O	1.93	0.52
2:B:50:VAL:CG2	2:B:51:THR:HG23	2.40	0.51
4:D:35:LEU:HB3	4:D:94:ALA:HB1	1.91	0.51
2:F:38:VAL:HG22	2:F:54:GLY:CA	2.41	0.51
1:A:12:PHE:C	1:A:12:PHE:HD1	2.18	0.51
1:E:123:ARG:HD2	1:E:126:LYS:CE	2.40	0.51
2:F:139:LYS:O	2:F:142:VAL:HG22	2.10	0.51
1:A:121:TRP:CB	1:A:128:VAL:HG22	2.41	0.51
1:A:147:LYS:HE3	1:A:149:HIS:CE1	2.45	0.51
2:B:36:GLU:O	2:B:50:VAL:CG2	2.58	0.51
4:D:39:GLU:CD	4:D:39:GLU:H	2.16	0.51
1:E:89:VAL:HG23	1:E:174:LEU:HD23	1.93	0.51
1:E:65:VAL:HB	3:G:313:THR:CG2	2.41	0.51
4:D:25:THR:OG1	4:D:28:GLU:HG3	2.10	0.51
2:F:145:THR:CG2	2:F:158:LEU:HB2	2.41	0.50
4:D:40:GLU:HG3	4:D:41:THR:HG23	1.94	0.50
1:E:118:ASN:HB3	1:E:166:GLU:HB2	1.93	0.50
2:B:109:LEU:HD12	2:B:109:LEU:N	2.27	0.50
2:F:116:VAL:HG22	2:F:160:MET:HG3	1.93	0.50
1:A:111:LYS:HG2	1:A:140:ARG:NH2	2.26	0.50
4:D:193:TYR:CE1	4:H:54:GLN:NE2	2.80	0.50
1:E:44:ARG:NE	1:E:135:THR:HG22	2.27	0.50
2:F:28:GLU:HB3	2:F:40:PHE:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:LEU:HD21	3:C:314:LEU:HD13	1.95	0.49
4:D:45:LEU:HD13	4:D:45:LEU:C	2.37	0.49
2:F:99:VAL:CG2	2:F:175:VAL:HG21	2.41	0.49
1:A:160:VAL:HG23	1:A:179:GLU:CB	2.42	0.49
1:E:23:MSE:HG2	1:E:24:PHE:N	2.27	0.49
1:A:23:MSE:HE3	1:A:23:MSE:C	2.37	0.49
4:H:134:LYS:NZ	4:H:172:ASN:HD22	2.09	0.49
4:H:60:PHE:HA	4:H:63:VAL:CG1	2.42	0.49
2:F:21:THR:O	2:F:80:ARG:NH1	2.43	0.49
2:B:93:ARG:NH1	2:B:153:TRP:O	2.46	0.49
4:H:15:PHE:HA	4:H:17:GLN:HE22	1.77	0.49
1:A:162:ASP:HB3	1:A:177:HIS:HA	1.94	0.49
4:D:136:VAL:O	4:D:140:LYS:HG3	2.12	0.49
1:E:111:LYS:HG2	1:E:140:ARG:NH2	2.28	0.48
1:A:21:GLU:OE2	1:A:136:VAL:HG22	2.13	0.48
2:B:10:GLN:HB2	2:B:31:ILE:HB	1.94	0.48
2:B:147:LEU:HD11	2:B:155:PHE:CD2	2.48	0.48
2:F:109:LEU:HD23	2:F:109:LEU:H	1.79	0.48
2:B:9:TRP:CH2	2:B:30:CYS:HB3	2.48	0.48
4:D:137:LYS:O	4:D:141:GLU:HG3	2.13	0.48
4:D:140:LYS:HE2	4:D:210:VAL:O	2.13	0.48
1:A:9:GLN:HG3	1:A:24:PHE:CE1	2.49	0.48
4:H:120:TYR:O	4:H:124:GLN:HG2	2.14	0.48
1:A:73:MSE:HG2	3:C:316:LEU:CD1	2.44	0.48
1:A:129:THR:O	1:A:130:THR:C	2.53	0.48
1:A:68:ALA:O	1:A:72:ILE:HG13	2.14	0.47
1:A:160:VAL:O	1:A:160:VAL:CG1	2.62	0.47
2:B:106:THR:HG23	2:B:110:GLN:HG3	1.95	0.47
2:F:93:ARG:NH2	2:F:153:TRP:O	2.46	0.47
4:H:62:ILE:HD12	4:H:79:MET:CE	2.44	0.47
4:H:152:ASP:O	4:H:158:VAL:HG21	2.14	0.47
1:E:95:SER:HB2	1:E:96:PRO:HD2	1.96	0.47
1:E:123:ARG:HB3	1:E:126:LYS:HE3	1.96	0.47
2:B:108:PRO:HG2	2:B:109:LEU:CD1	2.44	0.47
2:F:28:GLU:OE1	2:F:71:ARG:NE	2.47	0.47
2:F:68:LEU:O	2:F:72:ARG:HG3	2.15	0.47
1:E:101:GLU:O	1:E:102:PRO:C	2.57	0.47
1:A:174:LEU:HD23	1:A:175:LEU:N	2.29	0.47
2:B:177:HIS:CD2	2:B:178:PRO:HD2	2.49	0.47
2:B:177:HIS:CG	2:B:178:PRO:HD2	2.50	0.47
4:D:47:LEU:N	4:D:47:LEU:HD22	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:GLN:HG3	1:E:24:PHE:CE1	2.50	0.47
4:H:113:LYS:HZ3	4:H:117:ASP:CG	2.21	0.47
1:E:179:GLU:O	1:E:179:GLU:HG3	2.15	0.47
2:F:14:GLU:O	2:F:26:LEU:HD12	2.15	0.47
2:F:38:VAL:HG22	2:F:54:GLY:HA2	1.97	0.47
4:H:75:ILE:CD1	4:H:118:LEU:HA	2.45	0.47
1:A:69:ASN:OD1	3:C:316:LEU:HG	2.15	0.47
1:A:89:VAL:O	1:A:176:LYS:HE2	2.15	0.47
2:B:133:ARG:HD3	2:B:169:GLU:CD	2.40	0.47
1:A:67:LYS:NZ	4:D:88:ASP:OD1	2.48	0.47
4:D:156:GLY:HA2	4:D:188:TYR:OH	2.14	0.47
1:E:123:ARG:NH2	1:E:126:LYS:NZ	2.63	0.47
4:H:154:ARG:HG3	4:H:154:ARG:HH11	1.80	0.47
4:H:1:MET:CE	4:H:129:GLN:HA	2.45	0.46
2:F:110:GLN:HE21	2:F:111:HIS:N	2.08	0.46
4:H:159:ALA:CB	4:H:188:TYR:CE1	2.98	0.46
2:B:176:GLU:CG	2:B:183:PRO:HB3	2.44	0.46
2:F:97:PRO:HB3	2:F:122:PHE:HB3	1.97	0.46
2:B:187:GLU:OE1	2:B:189:ARG:NH1	2.49	0.46
1:A:90:THR:CG2	1:A:108:PHE:HB2	2.40	0.46
1:A:142:ASP:OD2	1:A:144:LEU:HD12	2.15	0.46
4:D:42:LYS:O	4:D:42:LYS:HG2	2.15	0.46
4:D:198:ILE:HD11	4:H:115:ASP:OD2	2.15	0.46
4:H:62:ILE:HD12	4:H:79:MET:HE1	1.98	0.46
4:H:51:LYS:CG	4:H:104:ILE:HG23	2.36	0.46
2:B:113:ASN:N	2:B:113:ASN:HD22	2.12	0.46
1:A:16:PRO:CD	2:B:6:ARG:HD2	2.37	0.46
1:A:89:VAL:CG2	1:A:165:VAL:HG21	2.46	0.46
1:E:103:ASN:OD1	1:E:104:VAL:N	2.48	0.46
2:B:25:ARG:HH21	2:B:27:LEU:CD2	2.27	0.45
2:B:166:ARG:HG3	2:B:169:GLU:OE2	2.16	0.45
4:D:200:LEU:O	4:D:203:THR:HB	2.15	0.45
2:F:81:HIS:HD2	3:G:309:VAL:HG22	1.81	0.45
1:A:123:ARG:NH2	1:A:161:TYR:CE2	2.85	0.45
1:A:129:THR:O	1:A:132:VAL:HG22	2.17	0.45
4:D:37:ASN:HD22	4:D:37:ASN:C	2.21	0.45
4:D:113:LYS:HE3	4:D:117:ASP:CG	2.42	0.45
1:E:105:LEU:HD12	1:E:151:LEU:HD23	1.97	0.45
4:H:201:LYS:HE2	4:H:211:PHE:O	2.16	0.45
2:F:70:GLN:OE1	2:F:71:ARG:NH2	2.49	0.45
1:E:124:ASN:HD21	1:E:159:ASP:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:88:SER:HA	2:B:92:GLN:HG3	1.99	0.45
2:B:107:GLN:NE2	2:B:110:GLN:HG2	2.32	0.45
4:D:37:ASN:ND2	4:D:38:LYS:N	2.57	0.45
4:H:1:MET:HE2	4:H:132:TRP:CE3	2.51	0.45
2:B:18:PHE:CD1	2:B:18:PHE:N	2.85	0.45
2:F:133:ARG:HG3	2:F:171:TYR:CE1	2.52	0.45
1:A:26:PHE:HB2	1:A:31:ILE:HD11	1.98	0.44
1:A:92:LEU:N	1:A:92:LEU:CD2	2.79	0.44
2:B:127:ILE:HG13	2:B:177:HIS:HB2	1.98	0.44
4:D:14:HIS:CD2	4:D:78:MET:SD	3.10	0.44
2:F:90:THR:OG1	2:F:91:VAL:N	2.50	0.44
2:F:106:THR:C	2:F:107:GLN:HG3	2.41	0.44
1:A:73:MSE:HG3	2:B:9:TRP:CZ3	2.52	0.44
1:A:123:ARG:NH2	1:A:161:TYR:OH	2.50	0.44
2:B:52:GLU:OE1	2:B:55:ARG:CZ	2.65	0.44
2:F:25:ARG:NH1	2:F:41:ASP:OD2	2.42	0.44
3:G:312:ASN:HB2	4:H:14:HIS:CE1	2.53	0.44
1:A:109:ILE:HD11	1:A:119:VAL:HG21	1.99	0.44
4:H:8:PRO:HG3	4:H:119:SER:HB3	1.98	0.44
4:D:170:ASP:OD1	4:D:172:ASN:HB2	2.17	0.44
1:A:11:GLU:HA	1:A:21:GLU:O	2.17	0.44
4:H:159:ALA:CB	4:H:187:VAL:HG21	2.48	0.44
1:A:160:VAL:CG2	1:A:179:GLU:HB3	2.47	0.44
2:B:52:GLU:OE2	2:B:55:ARG:NH1	2.51	0.44
2:B:70:GLN:OE1	2:B:70:GLN:C	2.60	0.44
1:E:79:TYR:N	1:E:79:TYR:CD1	2.85	0.44
2:F:36:GLU:OE2	2:F:39:ARG:NE	2.46	0.44
2:F:119:VAL:HG11	2:F:127:ILE:HD13	1.99	0.44
2:B:19:ASN:HD22	2:B:19:ASN:HA	1.65	0.43
3:C:317:ALA:O	3:C:318:THR:HG22	2.18	0.43
1:E:92:LEU:HD12	1:E:108:PHE:CZ	2.53	0.43
1:A:108:PHE:CD1	1:A:108:PHE:N	2.86	0.43
4:H:159:ALA:O	4:H:163:VAL:HG23	2.17	0.43
4:H:191:LYS:HE3	4:H:191:LYS:HA	2.00	0.43
1:A:84:ASN:HD22	1:A:114:PRO:HD2	1.82	0.43
2:B:88:SER:HA	2:B:92:GLN:CG	2.49	0.43
2:F:88:SER:O	2:F:92:GLN:HB2	2.19	0.43
4:H:57:ARG:NE	4:H:57:ARG:HA	2.33	0.43
2:F:10:GLN:HB2	2:F:31:ILE:HB	2.00	0.43
4:H:51:LYS:NZ	4:H:54:GLN:OE1	2.40	0.43
4:H:166:LEU:HB2	4:H:167:PHE:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:117:CYS:HB2	2:B:131:TRP:CZ2	2.54	0.43
4:H:167:PHE:C	4:H:169:SER:H	2.27	0.43
2:F:177:HIS:CG	2:F:178:PRO:HD2	2.53	0.43
4:H:142:MET:SD	4:H:187:VAL:HG12	2.58	0.43
1:A:76:ARG:NH1	3:C:317:ALA:HB3	2.34	0.43
2:B:147:LEU:HD11	2:B:155:PHE:HB3	2.01	0.43
4:D:143:LYS:HG2	4:H:50:LEU:HD21	2.01	0.43
1:E:124:ASN:N	1:E:124:ASN:HD22	2.16	0.43
4:H:191:LYS:HE3	4:H:191:LYS:O	2.18	0.43
4:D:53:ASN:N	4:D:53:ASN:HD22	2.17	0.43
2:F:99:VAL:HG12	2:F:186:VAL:HG21	1.99	0.43
1:A:23:MSE:HE2	1:A:23:MSE:HB3	1.95	0.42
4:D:93:GLU:HG3	4:D:99:GLN:HG2	2.00	0.42
2:F:170:VAL:HG13	2:F:170:VAL:O	2.19	0.42
4:D:47:LEU:H	4:D:47:LEU:CD2	2.32	0.42
1:E:26:PHE:HB2	1:E:31:ILE:HD11	2.01	0.42
1:A:15:ASN:ND2	1:A:70:LEU:HD12	2.33	0.42
2:B:70:GLN:OE1	2:B:70:GLN:O	2.37	0.42
4:D:149:GLN:NE2	4:D:162:LYS:NZ	2.68	0.42
2:F:177:HIS:CD2	2:F:178:PRO:HD2	2.54	0.42
1:E:62:ASN:HA	3:G:313:THR:CG2	2.48	0.42
1:A:101:GLU:O	1:A:102:PRO:C	2.61	0.42
2:B:31:ILE:N	2:B:31:ILE:HD12	2.34	0.42
4:H:85:VAL:O	4:H:88:ASP:HB2	2.19	0.42
1:E:69:ASN:CG	3:G:316:LEU:HG	2.44	0.42
2:B:114:LEU:H	2:B:114:LEU:CD2	2.31	0.42
4:D:43:GLU:O	4:D:47:LEU:HD23	2.19	0.42
4:D:99:GLN:NE2	4:D:102:ARG:HD2	2.34	0.42
1:E:123:ARG:NH2	1:E:126:LYS:HZ1	2.17	0.42
2:B:94:ARG:HH11	2:B:94:ARG:CG	2.27	0.42
4:D:45:LEU:HD13	4:D:45:LEU:O	2.19	0.42
2:F:107:GLN:CB	2:F:109:LEU:HD23	2.50	0.42
1:A:92:LEU:HD21	1:A:108:PHE:CE1	2.54	0.42
2:B:2:ASP:CG	2:B:6:ARG:HH22	2.28	0.42
4:D:14:HIS:N	4:D:74:GLU:OE1	2.50	0.42
1:E:3:GLU:HA	2:F:18:PHE:CD2	2.55	0.42
1:A:23:MSE:SE	1:A:25:ASP:HB2	2.70	0.42
2:B:4:ARG:HB2	2:B:6:ARG:NH1	2.35	0.41
2:B:27:LEU:HD12	2:B:29:ARG:CD	2.51	0.41
2:B:105:LYS:NZ	2:B:108:PRO:O	2.51	0.41
2:B:116:VAL:HG22	2:B:160:MET:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:ILE:HG12	2:F:14:GLU:HG2	2.02	0.41
1:E:11:GLU:HA	1:E:21:GLU:O	2.19	0.41
1:E:73:MSE:HG3	2:F:9:TRP:CZ3	2.55	0.41
2:F:27:LEU:HD12	2:F:29:ARG:HD3	2.02	0.41
2:F:67:LEU:HD21	3:G:314:LEU:CD2	2.48	0.41
1:A:86:PRO:HB3	1:A:169:GLY:O	2.20	0.41
2:B:142:VAL:HA	2:B:160:MET:O	2.20	0.41
4:D:17:GLN:CD	4:D:17:GLN:H	2.27	0.41
4:D:44:VAL:HA	4:D:47:LEU:HD23	2.02	0.41
1:A:13:TYR:OH	1:A:67:LYS:HE3	2.20	0.41
1:A:70:LEU:HD13	1:A:70:LEU:C	2.45	0.41
1:E:23:MSE:HB3	1:E:23:MSE:HE3	1.78	0.41
2:F:31:ILE:HD12	2:F:31:ILE:N	2.35	0.41
2:F:142:VAL:HA	2:F:160:MET:O	2.19	0.41
1:E:86:PRO:HB3	1:E:169:GLY:O	2.21	0.41
4:D:167:PHE:C	4:D:169:SER:H	2.29	0.41
4:D:203:THR:HG22	4:D:207:ALA:HB3	2.03	0.41
4:D:47:LEU:HD22	4:D:47:LEU:H	1.85	0.41
2:F:163:THR:O	2:F:165:PRO:HD3	2.20	0.41
4:H:154:ARG:HH11	4:H:154:ARG:CG	2.33	0.41
1:A:66:ASP:OD2	3:C:313:THR:HG21	2.20	0.41
1:A:92:LEU:CD2	1:A:108:PHE:CE1	3.03	0.41
4:D:2:LYS:HE2	4:D:2:LYS:CA	2.48	0.41
4:D:149:GLN:NE2	4:D:162:LYS:HZ1	2.19	0.41
4:D:157:GLU:O	4:D:161:ASN:ND2	2.54	0.41
2:F:134:ASN:HD22	2:F:170:VAL:CG1	2.34	0.41
2:B:161:LEU:HG	2:B:163:THR:HG23	2.03	0.41
1:E:175:LEU:C	1:E:175:LEU:HD23	2.46	0.41
2:F:94:ARG:HG3	2:F:94:ARG:NH1	2.34	0.41
4:H:93:GLU:HG3	4:H:99:GLN:HG2	2.01	0.41
1:E:70:LEU:HD13	2:F:9:TRP:CB	2.50	0.40
2:F:92:GLN:O	2:F:94:ARG:HG2	2.21	0.40
4:H:45:LEU:HD13	4:H:49:LYS:HE3	2.01	0.40
4:H:16:VAL:O	4:H:16:VAL:HG22	2.21	0.40
1:A:122:LEU:HD23	1:A:127:PRO:HA	2.02	0.40
2:B:152:ASP:OD2	2:B:152:ASP:C	2.63	0.40
4:D:62:ILE:HD12	4:D:79:MET:CE	2.52	0.40
4:D:203:THR:HG22	4:D:207:ALA:HB2	2.02	0.40
1:E:65:VAL:HB	3:G:313:THR:HG21	2.04	0.40
2:F:129:VAL:HG22	2:F:175:VAL:HG22	2.02	0.40
4:H:159:ALA:HB2	4:H:188:TYR:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:48:PHE:O	4:D:52:VAL:HG23	2.21	0.40
1:E:108:PHE:CD2	1:E:108:PHE:N	2.89	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2:LYS:NZ	1:E:2:LYS:NZ[3_655]	1.93	0.27

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	178/180 (99%)	163 (92%)	13 (7%)	2 (1%)	11	43
1	E	178/180 (99%)	163 (92%)	13 (7%)	2 (1%)	11	43
2	B	188/190 (99%)	171 (91%)	17 (9%)	0	100	100
2	F	188/190 (99%)	169 (90%)	19 (10%)	0	100	100
3	C	11/13 (85%)	9 (82%)	2 (18%)	0	100	100
3	G	11/13 (85%)	9 (82%)	2 (18%)	0	100	100
4	D	212/214 (99%)	201 (95%)	8 (4%)	3 (1%)	9	36
4	H	212/214 (99%)	201 (95%)	8 (4%)	3 (1%)	9	36
All	All	1178/1194 (99%)	1086 (92%)	82 (7%)	10 (1%)	16	50

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	PHE
1	E	180	PHE
4	H	168	GLY

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Mol	Chain	Res	Type
4	H	200	LEU
4	D	94	ALA
4	D	168	GLY
4	H	94	ALA
1	A	179	GLU
1	E	179	GLU
4	D	200	LEU

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	165/162 (102%)	154 (93%)	11 (7%)	15	46
1	E	165/162 (102%)	157 (95%)	8 (5%)	23	57
2	B	171/171 (100%)	157 (92%)	14 (8%)	10	37
2	F	171/171 (100%)	156 (91%)	15 (9%)	9	35
3	C	12/12 (100%)	11 (92%)	1 (8%)	10	37
3	G	11/12 (92%)	10 (91%)	1 (9%)	9	33
4	D	197/197 (100%)	179 (91%)	18 (9%)	9	33
4	H	197/197 (100%)	182 (92%)	15 (8%)	12	41
All	All	1089/1084 (100%)	1006 (92%)	83 (8%)	12	41

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	PHE
1	A	23	MSE
1	A	42	VAL
1	A	55	GLU
1	A	63	ILE
1	A	90	THR
1	A	92	LEU
1	A	128	VAL

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Mol	Chain	Res	Type
1	A	160	VAL
1	A	162	ASP
1	A	177	HIS
2	B	19	ASN
2	B	27	LEU
2	B	29	ARG
2	B	38	VAL
2	B	50	VAL
2	B	64	GLN
2	B	70	GLN
2	B	71	ARG
2	B	75	VAL
2	B	94	ARG
2	B	100	THR
2	B	129	VAL
2	B	133	ARG
2	B	166	ARG
3	C	318	THR
4	D	6	GLU
4	D	12	GLN
4	D	17	GLN
4	D	37	ASN
4	D	39	GLU
4	D	51	LYS
4	D	63	VAL
4	D	70	LEU
4	D	74	GLU
4	D	83	LEU
4	D	98	GLU
4	D	100	ILE
4	D	126	LYS
4	D	182	LEU
4	D	187	VAL
4	D	200	LEU
4	D	203	THR
4	D	212	GLU
1	E	42	VAL
1	E	47	GLU
1	E	78	ASN
1	E	88	GLU
1	E	90	THR
1	E	99	LEU

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Mol	Chain	Res	Type
1	E	102	PRO
1	E	177	HIS
2	F	3	THR
2	F	27	LEU
2	F	38	VAL
2	F	52	GLU
2	F	64	GLN
2	F	75	VAL
2	F	98	LYS
2	F	105	LYS
2	F	110	GLN
2	F	112	HIS
2	F	114	LEU
2	F	115	LEU
2	F	118	SER
2	F	143	VAL
2	F	166	ARG
3	G	314	LEU
4	H	17	GLN
4	H	27	LYS
4	H	42	LYS
4	H	45	LEU
4	H	63	VAL
4	H	70	LEU
4	H	74	GLU
4	H	83	LEU
4	H	107	LEU
4	H	145	LYS
4	H	153	LEU
4	H	160	ILE
4	H	182	LEU
4	H	187	VAL
4	H	191	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	94	ASN
1	A	149	HIS
1	A	177	HIS
2	B	19	ASN

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Mol	Chain	Res	Type
2	B	64	GLN
2	B	107	GLN
2	B	111	HIS
2	B	134	ASN
2	B	150	ASN
2	B	156	GLN
2	B	174	GLN
4	D	12	GLN
4	D	14	HIS
4	D	17	GLN
4	D	34	ASN
4	D	37	ASN
4	D	53	ASN
4	D	90	GLN
4	D	103	ASN
4	D	124	GLN
4	D	149	GLN
4	D	161	ASN
4	D	172	ASN
1	E	15	ASN
1	E	57	GLN
1	E	124	ASN
1	E	143	HIS
1	E	149	HIS
2	F	19	ASN
2	F	34	GLN
2	F	81	HIS
2	F	107	GLN
2	F	110	GLN
2	F	134	ASN
2	F	156	GLN
4	H	17	GLN
4	H	34	ASN
4	H	64	ASN
4	H	95	ASN
4	H	127	ASN
4	H	161	ASN
4	H	172	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	PO4	C	202	-	4,4,4	1.72	1 (25%)	6,6,6	0.45	0
5	PO4	H	214	-	4,4,4	1.79	2 (50%)	6,6,6	0.44	0
5	PO4	D	214	-	4,4,4	1.78	1 (25%)	6,6,6	0.50	0
5	PO4	E	204	-	4,4,4	1.73	2 (50%)	6,6,6	0.47	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	H	214	PO4	P-O4	-2.18	1.48	1.54
5	D	214	PO4	P-O4	-2.10	1.48	1.54
5	H	214	PO4	P-O3	-2.04	1.48	1.54
5	C	202	PO4	P-O2	-2.02	1.48	1.54
5	E	204	PO4	P-O3	-2.02	1.48	1.54
5	E	204	PO4	P-O2	-2.00	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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	177/180 (98%)	-0.30	3 (1%) 69 45	17, 31, 53, 78	0
1	E	177/180 (98%)	-0.37	2 (1%) 78 57	19, 32, 52, 81	0
2	B	190/190 (100%)	-0.12	7 (3%) 45 25	20, 34, 71, 95	0
2	F	190/190 (100%)	-0.12	7 (3%) 45 25	22, 36, 74, 94	0
3	C	13/13 (100%)	-0.48	0 100 100	23, 29, 37, 42	0
3	G	13/13 (100%)	0.10	1 (7%) 19 10	28, 31, 44, 49	0
4	D	214/214 (100%)	-0.19	4 (1%) 66 43	20, 36, 57, 67	0
4	H	214/214 (100%)	-0.14	2 (0%) 81 61	20, 38, 58, 73	0
All	All	1188/1194 (99%)	-0.20	26 (2%) 62 39	17, 34, 62, 95	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	109	LEU	4.1
2	F	112	HIS	3.4
2	B	111	HIS	3.1
2	F	108	PRO	2.9
1	A	181	ASP	2.8
4	H	199	GLU	2.8
2	B	109	LEU	2.7
2	B	108	PRO	2.7
2	B	164	VAL	2.6
4	D	6	GLU	2.6
2	B	112	HIS	2.5
1	A	180	PHE	2.3
2	F	1	GLY	2.2
2	B	168	GLY	2.2
2	F	164	VAL	2.2
4	D	21	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
4	D	199	GLU	2.2
3	G	318	THR	2.2
1	E	181	ASP	2.1
1	E	180	PHE	2.1
2	F	111	HIS	2.1
4	H	168	GLY	2.1
1	A	2	LYS	2.1
4	D	40	GLU	2.1
2	F	113	ASN	2.0
2	B	1	GLY	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 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PO4	E	204	5/5	0.93	0.11	67,68,69,69	0
5	PO4	C	202	5/5	0.95	0.11	59,59,60,61	0
5	PO4	H	214	5/5	0.96	0.09	51,51,52,53	0
5	PO4	D	214	5/5	0.97	0.07	41,42,42,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.