



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:03 AM UTC

PDB ID : 3CER / pdb_00003cer
Title : Crystal structure of the exopolyphosphatase-like protein Q8G5J2. Northeast Structural Genomics Consortium target BIR13
Authors : Kuzin, A.P.; Su, M.; Chen, Y.; Neely, H.; Seetharaman, J.; Shastry, R.; Fang, Y.; Cunningham, K.; Ma, L.-C.; Xiao, R.; Liu, J.; Baran, M.C.; Acton, T.B.; Rost, B.; Montelione, G.T.; Hunt, J.F.; Tong, L.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2008-02-29
Resolution : 2.40 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)

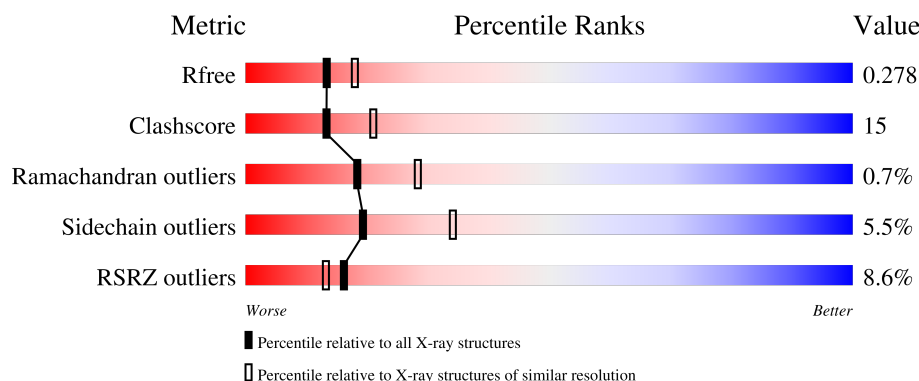
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	343	71% 23% • •
1	B	343	6% 71% 23% • •
1	C	343	2% 69% 24% 5% •
1	D	343	10% 65% 28% • •

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Validation Pipeline (wwPDB-VP) : 2.49

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Mol	Chain	Length	Quality of chain
1	E	343	 A horizontal bar chart showing the quality of chain E. The bar is divided into four segments: red (22%), green (60%), yellow (30%), and grey (6%). The segments are labeled with their respective percentages: 22%, 60%, 30%, and 6%.

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12990 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 Possible exopolyphosphatase-like protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	Se	0	0	0
			2516	1556	453	500	1	6			
1	B	330	Total	C	N	O	S	Se	0	0	0
			2516	1556	453	500	1	6			
1	C	333	Total	C	N	O	S	Se	0	0	0
			2539	1570	457	504	1	7			
1	D	330	Total	C	N	O	S	Se	0	0	0
			2515	1557	453	498	1	6			
1	E	322	Total	C	N	O	S	Se	0	0	0
			2458	1524	444	483	1	6			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP Q8G5J2
A	2	GLY	-	expression tag	UNP Q8G5J2
A	3	HIS	-	expression tag	UNP Q8G5J2
A	4	HIS	-	expression tag	UNP Q8G5J2
A	5	HIS	-	expression tag	UNP Q8G5J2
A	6	HIS	-	expression tag	UNP Q8G5J2
A	7	HIS	-	expression tag	UNP Q8G5J2
A	8	HIS	-	expression tag	UNP Q8G5J2
A	9	SER	-	expression tag	UNP Q8G5J2
A	10	HIS	-	expression tag	UNP Q8G5J2
A	260	PHE	LEU	engineered mutation	UNP Q8G5J2
A	276	ALA	VAL	engineered mutation	UNP Q8G5J2
B	1	MSE	-	expression tag	UNP Q8G5J2
B	2	GLY	-	expression tag	UNP Q8G5J2
B	3	HIS	-	expression tag	UNP Q8G5J2
B	4	HIS	-	expression tag	UNP Q8G5J2
B	5	HIS	-	expression tag	UNP Q8G5J2
B	6	HIS	-	expression tag	UNP Q8G5J2
B	7	HIS	-	expression tag	UNP Q8G5J2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	8	HIS	-	expression tag	UNP Q8G5J2
B	9	SER	-	expression tag	UNP Q8G5J2
B	10	HIS	-	expression tag	UNP Q8G5J2
B	260	PHE	LEU	engineered mutation	UNP Q8G5J2
B	276	ALA	VAL	engineered mutation	UNP Q8G5J2
C	1	MSE	-	expression tag	UNP Q8G5J2
C	2	GLY	-	expression tag	UNP Q8G5J2
C	3	HIS	-	expression tag	UNP Q8G5J2
C	4	HIS	-	expression tag	UNP Q8G5J2
C	5	HIS	-	expression tag	UNP Q8G5J2
C	6	HIS	-	expression tag	UNP Q8G5J2
C	7	HIS	-	expression tag	UNP Q8G5J2
C	8	HIS	-	expression tag	UNP Q8G5J2
C	9	SER	-	expression tag	UNP Q8G5J2
C	10	HIS	-	expression tag	UNP Q8G5J2
C	260	PHE	LEU	engineered mutation	UNP Q8G5J2
C	276	ALA	VAL	engineered mutation	UNP Q8G5J2
D	1	MSE	-	expression tag	UNP Q8G5J2
D	2	GLY	-	expression tag	UNP Q8G5J2
D	3	HIS	-	expression tag	UNP Q8G5J2
D	4	HIS	-	expression tag	UNP Q8G5J2
D	5	HIS	-	expression tag	UNP Q8G5J2
D	6	HIS	-	expression tag	UNP Q8G5J2
D	7	HIS	-	expression tag	UNP Q8G5J2
D	8	HIS	-	expression tag	UNP Q8G5J2
D	9	SER	-	expression tag	UNP Q8G5J2
D	10	HIS	-	expression tag	UNP Q8G5J2
D	260	PHE	LEU	engineered mutation	UNP Q8G5J2
D	276	ALA	VAL	engineered mutation	UNP Q8G5J2
E	1	MSE	-	expression tag	UNP Q8G5J2
E	2	GLY	-	expression tag	UNP Q8G5J2
E	3	HIS	-	expression tag	UNP Q8G5J2
E	4	HIS	-	expression tag	UNP Q8G5J2
E	5	HIS	-	expression tag	UNP Q8G5J2
E	6	HIS	-	expression tag	UNP Q8G5J2
E	7	HIS	-	expression tag	UNP Q8G5J2
E	8	HIS	-	expression tag	UNP Q8G5J2
E	9	SER	-	expression tag	UNP Q8G5J2
E	10	HIS	-	expression tag	UNP Q8G5J2
E	260	PHE	LEU	engineered mutation	UNP Q8G5J2
E	276	ALA	VAL	engineered mutation	UNP Q8G5J2

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

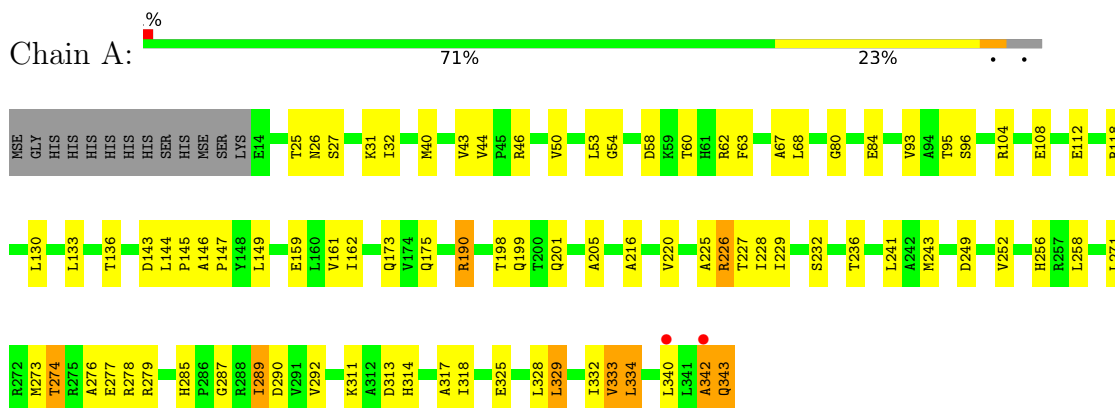
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	122	Total	O	0	0
			122	122		
3	B	36	Total	O	0	0
			36	36		
3	C	167	Total	O	0	0
			167	167		
3	D	29	Total	O	0	0
			29	29		
3	E	12	Total	O	0	0
			12	12		

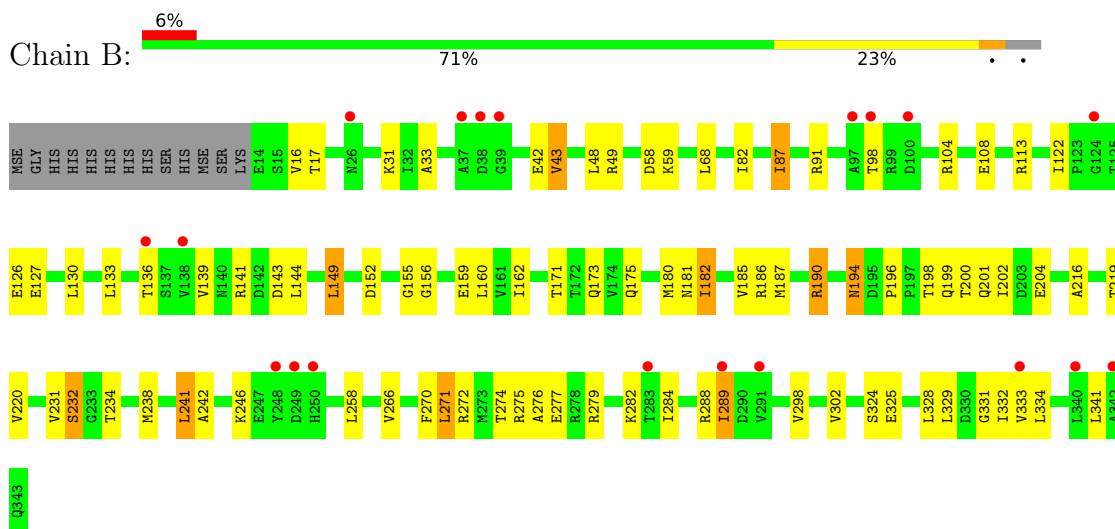
3 Residue-property plots [i](#)

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.

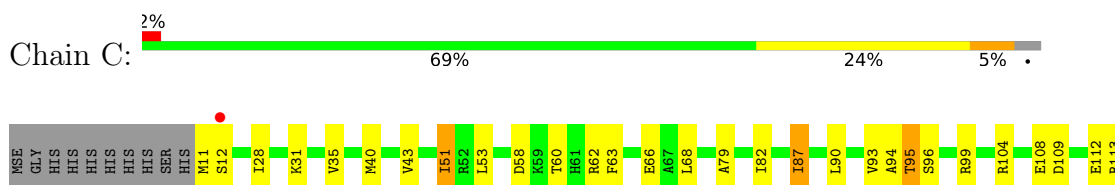
- Molecule 1: Possible exopolyphosphatase-like protein

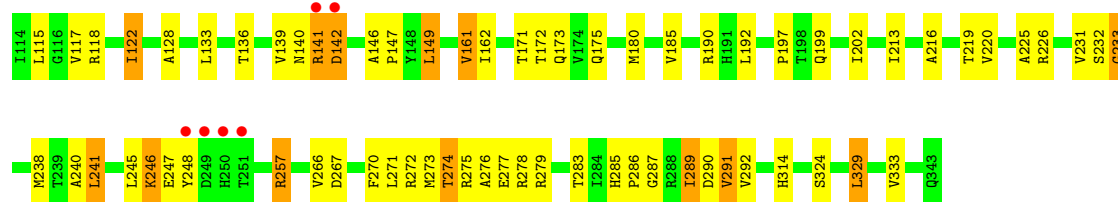


- Molecule 1: Possible exopolyphosphatase-like protein



- Molecule 1: Possible exopolyphosphatase-like protein

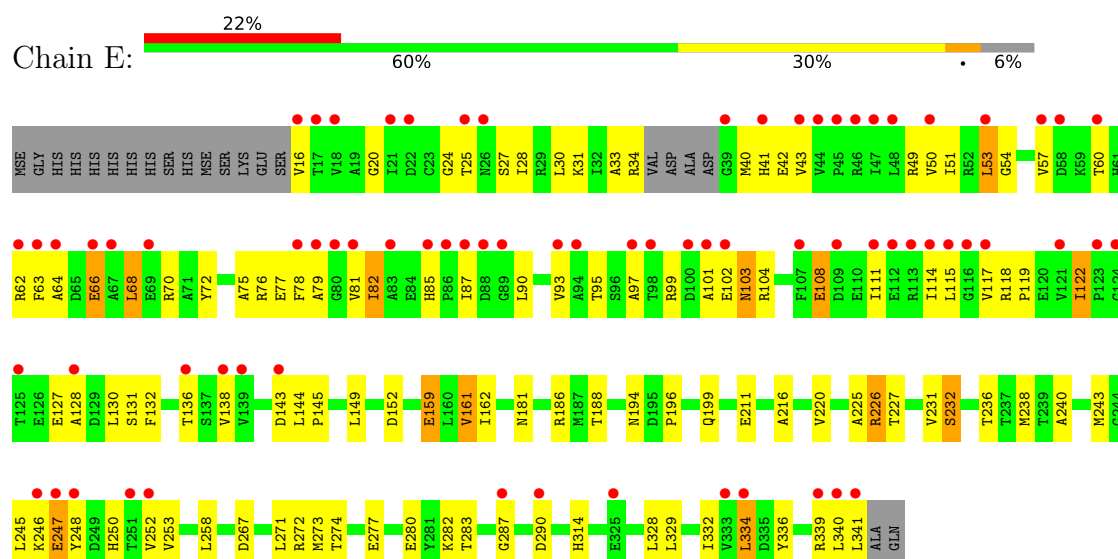




• Molecule 1: Possible exopolyphosphatase-like protein



• Molecule 1: Possible exopolyphosphatase-like protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	83.64Å 307.36Å 179.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 2.40 19.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.5 (19.90-2.40) 96.9 (19.90-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.09 (at 2.39Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.221 , 0.267 0.236 , 0.278	Depositor DCC
R_{free} test set	8653 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.314	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12990	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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: 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	0.47	0/2547	0.95	6/3443 (0.2%)
1	B	0.40	0/2547	0.86	3/3443 (0.1%)
1	C	0.50	0/2570	0.98	11/3472 (0.3%)
1	D	0.37	0/2546	0.87	3/3442 (0.1%)
1	E	0.35	0/2488	0.85	4/3362 (0.1%)
All	All	0.42	0/12698	0.90	27/17162 (0.2%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	95	THR	N-CA-C	10.87	119.19	108.75
1	C	43	VAL	N-CA-C	-9.40	102.74	111.67
1	A	43	VAL	N-CA-C	-9.32	104.29	112.12
1	D	291	VAL	N-CA-C	9.04	119.96	111.91
1	C	95	THR	N-CA-C	8.80	117.20	108.75
1	E	66	GLU	N-CA-C	-7.77	103.76	113.55
1	C	233	GLY	N-CA-C	7.65	121.90	112.64
1	A	226	ARG	N-CA-C	-6.71	105.66	114.31
1	C	291	VAL	N-CA-C	6.50	119.40	113.10
1	C	226	ARG	N-CA-C	-5.98	106.96	114.56
1	C	94	ALA	CA-C-N	-5.76	116.97	123.13
1	C	94	ALA	C-N-CA	-5.76	116.97	123.13
1	B	289	ILE	N-CA-C	5.68	117.10	110.62
1	E	27	SER	N-CA-C	5.54	115.86	108.38
1	A	96	SER	N-CA-C	5.49	117.72	111.02
1	A	67	ALA	N-CA-C	-5.42	105.29	111.14
1	B	43	VAL	N-CA-C	-5.39	107.57	112.96
1	C	225	ALA	N-CA-C	5.39	117.68	110.35
1	C	96	SER	N-CA-C	5.29	120.04	111.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	252	VAL	N-CA-C	5.26	120.28	109.34
1	D	43	VAL	N-CA-C	-5.21	107.08	111.56
1	C	289	ILE	N-CA-C	5.21	115.83	110.36
1	E	211	GLU	N-CA-C	-5.20	105.52	111.14
1	C	99	ARG	N-CA-C	-5.17	105.65	111.28
1	A	205	ALA	N-CA-C	-5.16	105.11	111.40
1	B	182	ILE	N-CA-C	5.04	116.25	108.44
1	E	82	ILE	N-CA-C	-5.02	106.24	113.07

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	2516	0	2470	56	0
1	B	2516	0	2470	68	0
1	C	2539	0	2497	79	0
1	D	2515	0	2475	79	0
1	E	2458	0	2423	91	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
2	C	20	0	0	1	0
2	D	15	0	0	0	0
2	E	15	0	0	0	0
3	A	122	0	0	2	0
3	B	36	0	0	0	0
3	C	167	0	0	2	0
3	D	29	0	0	0	0
3	E	12	0	0	0	0
All	All	12990	0	12335	370	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 15.

All (370) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:ILE:HD13	1:A:318:ILE:HG21	1.36	1.06
1:C:60:THR:HG22	1:C:62:ARG:HG2	1.38	1.02
1:C:279:ARG:HG2	1:C:289:ILE:HD13	1.40	1.00
1:D:173:GLN:HE21	1:D:175:GLN:HE22	1.05	0.98
1:B:173:GLN:HE21	1:B:175:GLN:HE22	1.09	0.98
1:B:196:PRO:HD3	1:B:274:THR:HG22	1.48	0.92
1:A:274:THR:HG22	1:A:277:GLU:H	1.35	0.90
1:A:285:HIS:HD2	1:A:287:GLY:H	1.23	0.86
1:C:285:HIS:HD2	1:C:287:GLY:H	1.22	0.84
1:E:152:ASP:HB3	1:E:159:GLU:HG2	1.60	0.83
1:D:63:PHE:HB2	1:D:103:ASN:HD21	1.43	0.83
1:E:199:GLN:HE22	1:E:272:ARG:HH22	1.28	0.81
1:C:31:LYS:HE2	1:C:40:MSE:HE1	1.63	0.80
1:C:173:GLN:HE21	1:C:175:GLN:HE22	1.31	0.79
1:C:274:THR:HG22	1:C:277:GLU:H	1.45	0.79
1:E:93:VAL:HG21	1:E:332:ILE:HD12	1.66	0.78
1:C:238:MSE:HE2	1:C:267:ASP:HA	1.65	0.78
1:B:274:THR:OG1	1:B:277:GLU:HG3	1.85	0.77
1:A:173:GLN:HE21	1:A:175:GLN:HE22	1.29	0.77
1:C:238:MSE:HE3	1:C:266:VAL:HG13	1.65	0.76
1:A:93:VAL:HG21	1:A:332:ILE:HD12	1.67	0.76
1:B:152:ASP:HB3	1:B:159:GLU:HG2	1.67	0.76
1:C:257:ARG:HH11	1:C:257:ARG:HB2	1.51	0.75
1:A:60:THR:HG22	1:A:62:ARG:HG2	1.67	0.75
1:B:231:VAL:O	1:B:232:SER:HB2	1.86	0.75
1:B:82:ILE:HG23	1:B:87:ILE:HD12	1.70	0.74
1:C:199:GLN:NE2	1:C:272:ARG:HH12	1.86	0.74
1:E:50:VAL:HG21	1:E:287:GLY:HA3	1.70	0.74
1:A:279:ARG:HG2	1:A:289:ILE:HD13	1.70	0.73
1:E:79:ALA:HB2	1:E:115:LEU:HD23	1.68	0.73
1:E:16:VAL:HG11	1:E:340:LEU:HD12	1.70	0.73
1:E:199:GLN:NE2	1:E:272:ARG:HH12	1.87	0.73
1:E:63:PHE:H	1:E:103:ASN:HD21	1.37	0.73
1:D:173:GLN:NE2	1:D:175:GLN:HE22	1.86	0.72
1:B:241:LEU:HG	1:B:270:PHE:CZ	2.24	0.72
1:A:328:LEU:O	1:A:332:ILE:HG12	1.90	0.71
1:D:51:ILE:HD13	1:D:51:ILE:H	1.56	0.71
1:D:173:GLN:HE21	1:D:175:GLN:NE2	1.85	0.71
1:B:194:ASN:HD22	1:B:194:ASN:N	1.86	0.70
1:E:25:THR:OG1	1:E:97:ALA:HB2	1.91	0.70
1:B:113:ARG:HH11	1:B:113:ARG:HG2	1.55	0.70
1:C:95:THR:HG22	1:C:122:ILE:HD11	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:ARG:HD3	1:C:141:ARG:H	1.56	0.69
1:E:60:THR:HG22	1:E:62:ARG:HG2	1.73	0.69
1:C:274:THR:HG22	1:C:277:GLU:HG3	1.75	0.69
1:E:250:HIS:HA	1:E:253:VAL:HG12	1.74	0.69
1:B:173:GLN:NE2	1:B:175:GLN:HE22	1.88	0.68
1:D:93:VAL:HG21	1:D:332:ILE:HD12	1.75	0.68
1:D:109:ASP:HA	1:D:118:ARG:NH1	2.08	0.68
1:D:87:ILE:HD13	1:D:87:ILE:H	1.58	0.68
1:C:51:ILE:HD13	1:C:51:ILE:H	1.59	0.68
1:C:11:MSE:HG2	1:C:12:SER:H	1.59	0.67
1:D:130:LEU:HD13	1:D:332:ILE:HD13	1.77	0.67
1:C:60:THR:CG2	1:C:62:ARG:HG2	2.18	0.66
1:C:128:ALA:HB1	1:C:161:VAL:HG22	1.77	0.66
1:B:98:THR:HG22	1:B:104:ARG:HG3	1.76	0.66
1:A:146:ALA:H	1:C:199:GLN:NE2	1.94	0.65
1:D:216:ALA:O	1:D:220:VAL:HG12	1.95	0.65
1:E:199:GLN:HE22	1:E:272:ARG:NH2	1.94	0.65
1:A:243:MSE:HE1	1:A:252:VAL:HG22	1.78	0.65
1:D:132:PHE:O	1:D:136:THR:HG22	1.97	0.65
1:B:279:ARG:HG2	1:B:289:ILE:HD13	1.78	0.64
1:B:160:LEU:HD11	1:B:180:MSE:HE2	1.80	0.64
1:B:202:ILE:HD12	1:B:271:LEU:HD11	1.80	0.63
1:B:241:LEU:HD11	1:B:284:ILE:HD11	1.79	0.63
1:B:198:THR:O	1:B:202:ILE:HG12	1.98	0.63
1:E:341:LEU:H	1:E:341:LEU:HD23	1.64	0.63
1:C:285:HIS:CD2	1:C:287:GLY:H	2.11	0.62
1:C:247:GLU:C	1:C:283:THR:HG22	2.24	0.62
1:E:108:GLU:HA	1:E:119:PRO:HG2	1.80	0.62
1:B:173:GLN:HE21	1:B:175:GLN:NE2	1.91	0.62
1:C:140:ASN:HD21	1:C:142:ASP:HB3	1.65	0.62
1:C:274:THR:CG2	1:C:277:GLU:H	2.11	0.62
1:C:257:ARG:HB2	1:C:257:ARG:NH1	2.15	0.61
1:A:147:PRO:HD2	1:A:226:ARG:HG3	1.82	0.61
1:A:173:GLN:HE21	1:A:175:GLN:NE2	1.97	0.61
1:E:243:MSE:HE1	1:E:252:VAL:HG12	1.83	0.61
1:C:180:MSE:SE	1:C:213:ILE:HD13	2.51	0.61
1:E:87:ILE:HD12	1:E:87:ILE:O	2.00	0.60
1:C:241:LEU:HG	1:C:270:PHE:CZ	2.36	0.60
1:C:171:THR:HG23	1:C:172:THR:HG23	1.82	0.60
1:D:31:LYS:CB	1:D:329:LEU:HD11	2.32	0.60
1:E:247:GLU:O	1:E:283:THR:HA	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:MSE:HE2	1:E:267:ASP:HA	1.83	0.60
1:C:93:VAL:HG13	1:C:122:ILE:HD12	1.83	0.60
1:D:185:VAL:HA	1:D:291:VAL:HG11	1.84	0.59
1:E:33:ALA:HA	1:E:43:VAL:HG23	1.84	0.59
1:E:128:ALA:HB1	1:E:161:VAL:HG22	1.85	0.59
1:D:63:PHE:HB3	1:D:68:LEU:HD13	1.83	0.59
1:D:40:MSE:HE3	1:D:138:VAL:HG22	1.85	0.59
1:C:122:ILE:HD13	1:C:122:ILE:H	1.68	0.59
1:A:80:GLY:O	1:A:84:GLU:HG3	2.03	0.59
1:E:196:PRO:HD3	1:E:274:THR:HG22	1.84	0.59
1:B:152:ASP:HB3	1:B:159:GLU:CG	2.33	0.58
1:D:231:VAL:HG12	1:D:324:SER:HB3	1.85	0.58
1:D:231:VAL:O	1:D:232:SER:HB2	2.04	0.58
1:D:31:LYS:HB2	1:D:329:LEU:HD11	1.84	0.58
1:E:103:ASN:N	1:E:103:ASN:HD22	1.99	0.58
1:E:216:ALA:O	1:E:220:VAL:HG12	2.02	0.58
1:A:329:LEU:O	1:A:333:VAL:HG12	2.04	0.57
1:A:130:LEU:HD13	1:A:332:ILE:HD13	1.86	0.57
1:C:248:TYR:N	1:C:283:THR:HG22	2.20	0.57
1:D:109:ASP:HA	1:D:118:ARG:HH12	1.69	0.56
1:A:228:ILE:CD1	1:A:318:ILE:HG21	2.22	0.56
1:B:216:ALA:O	1:B:220:VAL:HG12	2.06	0.56
1:B:133:LEU:HD12	1:B:331:GLY:HA2	1.87	0.56
1:C:139:VAL:HG22	3:C:466:HOH:O	2.06	0.56
1:C:141:ARG:H	1:C:141:ARG:CD	2.19	0.56
1:D:128:ALA:HB1	1:D:161:VAL:HG22	1.87	0.56
1:E:130:LEU:HD23	1:E:332:ILE:HD13	1.87	0.56
1:A:25:THR:HG23	1:A:54:GLY:HA3	1.87	0.56
1:E:240:ALA:HB1	1:E:245:LEU:HD12	1.88	0.55
1:E:328:LEU:O	1:E:332:ILE:HG12	2.07	0.55
1:E:132:PHE:O	1:E:136:THR:HG22	2.06	0.55
1:E:194:ASN:N	1:E:194:ASN:HD22	2.05	0.55
1:C:231:VAL:HG12	1:C:324:SER:HB3	1.89	0.55
1:E:31:LYS:HE3	1:E:42:GLU:HG2	1.90	0.54
1:B:276:ALA:HA	1:B:279:ARG:NH1	2.22	0.54
1:D:31:LYS:C	1:D:32:ILE:HD12	2.32	0.54
1:E:62:ARG:HA	1:E:101:ALA:HB1	1.89	0.54
1:B:198:THR:OG1	1:B:201:GLN:HG3	2.07	0.54
1:B:194:ASN:N	1:B:194:ASN:ND2	2.55	0.54
1:C:122:ILE:H	1:C:122:ILE:CD1	2.21	0.54
1:E:99:ARG:HH11	1:E:99:ARG:HB2	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:ARG:HD3	1:C:141:ARG:N	2.23	0.53
1:A:273:MSE:HG2	1:A:277:GLU:HB2	1.91	0.53
1:E:77:GLU:O	1:E:81:VAL:HG23	2.08	0.53
1:E:64:ALA:HB1	1:E:66:GLU:OE2	2.09	0.53
1:E:78:PHE:O	1:E:82:ILE:HG12	2.09	0.53
1:A:279:ARG:CG	1:A:289:ILE:HD13	2.37	0.52
1:A:285:HIS:CD2	1:A:287:GLY:H	2.14	0.52
1:B:16:VAL:HG13	1:B:341:LEU:HD21	1.90	0.52
1:B:113:ARG:HG2	1:B:113:ARG:NH1	2.23	0.52
1:D:196:PRO:HD3	1:D:274:THR:HG22	1.91	0.52
1:E:31:LYS:HB2	1:E:329:LEU:HD21	1.92	0.52
1:D:29:ARG:HD3	1:D:46:ARG:HD2	1.92	0.52
1:D:285:HIS:CD2	1:D:287:GLY:H	2.27	0.52
1:E:93:VAL:CG1	1:E:122:ILE:HD12	2.40	0.52
1:A:58:ASP:OD2	1:A:190:ARG:HD3	2.09	0.52
1:C:274:THR:HG23	1:C:276:ALA:N	2.25	0.52
1:C:238:MSE:HE2	1:C:267:ASP:OD1	2.10	0.52
1:E:226:ARG:HG3	1:E:226:ARG:HH11	1.74	0.52
1:E:231:VAL:O	1:E:232:SER:HB3	2.09	0.52
1:D:234:THR:O	1:D:238:MSE:HG2	2.09	0.51
1:E:51:ILE:O	1:E:70:ARG:HD2	2.11	0.51
1:C:274:THR:CG2	1:C:277:GLU:HG3	2.39	0.51
1:C:199:GLN:HE22	1:C:272:ARG:HH12	1.58	0.51
1:E:50:VAL:HG13	1:E:50:VAL:O	2.10	0.51
1:C:199:GLN:HE22	1:C:272:ARG:HH22	1.58	0.51
1:C:233:GLY:HA3	2:C:346:SO4:O3	2.10	0.51
1:B:234:THR:O	1:B:238:MSE:HG2	2.10	0.51
1:C:35:VAL:HG22	1:C:40:MSE:HB3	1.92	0.51
1:C:238:MSE:CE	1:C:267:ASP:HA	2.39	0.51
1:D:304:ALA:O	1:D:308:GLU:HG3	2.11	0.51
1:E:188:THR:HG21	1:E:290:ASP:O	2.10	0.51
1:C:113:ARG:HG3	1:C:113:ARG:HH11	1.76	0.51
1:C:278:ARG:HD3	1:C:292:VAL:HG21	1.92	0.51
1:D:108:GLU:HG2	1:D:119:PRO:HG2	1.92	0.51
1:D:195:ASP:CG	1:D:275:ARG:HG3	2.36	0.51
1:C:275:ARG:HD2	1:C:290:ASP:HA	1.93	0.51
1:A:274:THR:HG23	1:A:276:ALA:H	1.77	0.50
1:E:127:GLU:O	1:E:131:SER:HB2	2.11	0.50
1:B:136:THR:O	1:B:139:VAL:HG22	2.11	0.50
1:E:132:PHE:HB2	1:E:161:VAL:HG11	1.93	0.50
1:B:58:ASP:HB2	1:B:59:LYS:NZ	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:GLN:NE2	1:A:175:GLN:HE22	2.04	0.50
1:B:242:ALA:HA	1:B:266:VAL:HG11	1.93	0.50
1:C:87:ILE:HD13	1:C:87:ILE:H	1.75	0.50
1:A:32:ILE:HD12	1:A:44:VAL:HG21	1.93	0.50
1:B:104:ARG:HD3	1:B:108:GLU:OE1	2.11	0.50
1:B:48:LEU:HD21	1:B:288:ARG:NH2	2.27	0.50
1:C:66:GLU:H	1:C:66:GLU:CD	2.19	0.50
1:E:76:ARG:HA	1:E:114:ILE:HG21	1.94	0.50
1:D:56:ASP:HA	1:D:189:GLU:OE1	2.12	0.49
1:E:149:LEU:HD23	1:E:162:ILE:HB	1.93	0.49
1:E:232:SER:O	1:E:236:THR:HG22	2.12	0.49
1:D:110:GLU:O	1:D:114:ILE:HG12	2.11	0.49
1:E:34:ARG:HG2	1:E:41:HIS:HB2	1.94	0.49
1:B:87:ILE:HD13	1:B:87:ILE:H	1.77	0.49
1:D:94:ALA:HB1	1:D:98:THR:OG1	2.12	0.49
1:E:108:GLU:HG2	1:E:119:PRO:HB2	1.93	0.49
1:E:250:HIS:HA	1:E:253:VAL:CG1	2.42	0.49
1:D:19:ALA:HB2	1:D:32:ILE:HG13	1.93	0.49
1:D:181:ASN:HB3	1:D:186:ARG:NH1	2.27	0.49
1:D:288:ARG:O	1:D:292:VAL:HG23	2.13	0.49
1:B:200:THR:O	1:B:204:GLU:HG3	2.12	0.49
1:D:50:VAL:HG21	1:D:285:HIS:CD2	2.48	0.49
1:D:237:THR:O	1:D:241:LEU:HD13	2.12	0.49
1:E:103:ASN:ND2	1:E:103:ASN:H	2.11	0.49
1:C:113:ARG:HG3	1:C:113:ARG:NH1	2.28	0.48
1:B:202:ILE:CD1	1:B:271:LEU:HD11	2.44	0.48
1:A:311:LYS:HE3	1:A:317:ALA:HB2	1.94	0.48
1:B:246:LYS:O	1:B:282:LYS:HB2	2.13	0.48
1:D:51:ILE:H	1:D:51:ILE:CD1	2.23	0.48
1:E:181:ASN:HB3	1:E:186:ARG:HH11	1.77	0.48
1:B:325:GLU:OE1	1:B:325:GLU:HA	2.13	0.48
1:C:192:LEU:HD22	1:C:202:ILE:HD13	1.95	0.48
1:C:274:THR:HG23	1:C:276:ALA:H	1.76	0.48
1:B:333:VAL:HG23	1:B:334:LEU:N	2.29	0.48
1:C:146:ALA:HB1	1:C:147:PRO:HA	1.95	0.48
1:A:340:LEU:C	1:A:342:ALA:H	2.21	0.48
1:C:216:ALA:O	1:C:220:VAL:HG12	2.13	0.48
1:A:32:ILE:HB	1:A:44:VAL:HG23	1.95	0.47
1:B:98:THR:CG2	1:B:104:ARG:HG3	2.44	0.47
1:A:274:THR:HB	1:A:277:GLU:OE1	2.13	0.47
1:C:273:MSE:HG2	1:C:277:GLU:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:293:GLY:O	1:D:297:VAL:HG23	2.14	0.47
1:B:144:LEU:N	1:B:144:LEU:HD12	2.29	0.47
1:C:240:ALA:HB1	1:C:245:LEU:HD12	1.95	0.47
1:D:31:LYS:HE3	1:D:42:GLU:HG3	1.96	0.47
1:E:103:ASN:HD22	1:E:103:ASN:H	1.63	0.47
1:E:117:VAL:HG12	1:E:118:ARG:H	1.79	0.47
1:A:343:GLN:HE21	1:A:343:GLN:HB3	1.57	0.47
1:B:122:ILE:HD12	1:B:122:ILE:O	2.14	0.47
1:B:242:ALA:CA	1:B:266:VAL:HG11	2.44	0.47
1:E:103:ASN:N	1:E:103:ASN:ND2	2.62	0.47
1:A:313:ASP:OD2	1:A:314:HIS:HD2	1.96	0.47
1:B:231:VAL:HG12	1:B:324:SER:HB3	1.97	0.47
1:D:50:VAL:HG11	1:D:287:GLY:HA3	1.96	0.47
1:D:250:HIS:O	1:D:253:VAL:HG22	2.15	0.47
1:D:215:GLU:HG3	1:D:218:ARG:NH2	2.29	0.47
1:B:17:THR:O	1:B:87:ILE:HB	2.15	0.46
1:D:286:PRO:HA	1:D:289:ILE:HD13	1.97	0.46
1:E:99:ARG:HB2	1:E:99:ARG:NH1	2.30	0.46
1:E:108:GLU:HB3	1:E:119:PRO:HD2	1.97	0.46
1:C:58:ASP:OD2	1:C:190:ARG:HD3	2.15	0.46
1:A:216:ALA:O	1:A:220:VAL:HG12	2.15	0.46
1:A:249:ASP:O	1:A:252:VAL:HG12	2.16	0.46
1:E:63:PHE:HB3	1:E:68:LEU:HD13	1.98	0.46
1:E:277:GLU:O	1:E:280:GLU:HB2	2.15	0.46
1:B:186:ARG:O	1:B:190:ARG:HB2	2.15	0.46
1:D:258:LEU:HD22	1:D:262:ASP:HB2	1.97	0.46
1:C:31:LYS:HB2	1:C:329:LEU:CD1	2.46	0.46
1:A:27:SER:HB3	1:A:50:VAL:HA	1.97	0.46
1:B:155:GLY:O	1:B:185:VAL:HB	2.15	0.46
1:A:60:THR:CG2	1:A:62:ARG:HG2	2.41	0.46
1:C:79:ALA:HB2	1:C:115:LEU:HD23	1.97	0.46
1:A:31:LYS:HD3	1:A:333:VAL:HG11	1.98	0.46
1:E:226:ARG:HH12	1:E:314:HIS:CE1	2.34	0.46
1:E:250:HIS:CA	1:E:253:VAL:HG12	2.44	0.46
1:C:149:LEU:HD23	1:C:162:ILE:HB	1.98	0.45
1:E:226:ARG:HG3	1:E:226:ARG:NH1	2.32	0.45
1:C:82:ILE:HD13	1:C:90:LEU:HD22	1.99	0.45
1:B:182:ILE:C	1:B:182:ILE:HD12	2.42	0.45
1:D:275:ARG:HG2	1:D:275:ARG:HH11	1.81	0.45
1:D:158:THR:HB	1:D:182:ILE:HD11	1.98	0.45
1:D:251:THR:O	1:D:253:VAL:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:LEU:HD22	1:E:63:PHE:CE1	2.52	0.45
1:B:328:LEU:O	1:B:332:ILE:HG13	2.16	0.45
1:D:104:ARG:O	1:D:108:GLU:HG3	2.16	0.45
1:A:112:GLU:CD	1:A:118:ARG:HD2	2.42	0.45
1:A:104:ARG:O	1:A:108:GLU:HG3	2.17	0.45
1:C:314:HIS:HE1	3:C:419:HOH:O	2.00	0.45
1:D:254:ASP:HB2	1:D:325:GLU:HG2	1.99	0.45
1:E:246:LYS:O	1:E:282:LYS:HB3	2.17	0.45
1:E:341:LEU:H	1:E:341:LEU:CD2	2.29	0.45
1:A:149:LEU:HD23	1:A:162:ILE:HB	1.99	0.45
1:E:226:ARG:HH12	1:E:314:HIS:CG	2.35	0.45
1:A:146:ALA:H	1:C:199:GLN:HE21	1.64	0.44
1:B:156:GLY:O	1:B:186:ARG:HD2	2.16	0.44
1:A:311:LYS:CE	1:A:317:ALA:HB2	2.48	0.44
1:C:274:THR:HG22	1:C:277:GLU:N	2.25	0.44
1:D:26:ASN:O	1:D:50:VAL:HG13	2.18	0.44
1:E:231:VAL:O	1:E:232:SER:CB	2.66	0.44
1:B:141:ARG:H	1:B:141:ARG:HD2	1.81	0.44
1:C:238:MSE:CE	1:C:266:VAL:HG13	2.42	0.44
1:A:279:ARG:NH2	3:A:395:HOH:O	2.49	0.44
1:E:117:VAL:HG12	1:E:118:ARG:N	2.33	0.44
1:C:241:LEU:HG	1:C:270:PHE:CE2	2.53	0.44
1:D:29:ARG:HA	1:D:47:ILE:O	2.18	0.44
1:E:72:TYR:HA	1:E:75:ALA:HB3	1.99	0.44
1:E:273:MSE:HG2	1:E:277:GLU:HB3	1.99	0.44
1:D:59:LYS:HG3	1:D:60:THR:N	2.32	0.43
1:D:182:ILE:HD13	1:D:182:ILE:H	1.83	0.43
1:E:24:GLY:HA2	1:E:95:THR:OG1	2.18	0.43
1:C:122:ILE:HD13	1:C:122:ILE:N	2.30	0.43
1:D:195:ASP:OD1	1:D:275:ARG:HG3	2.18	0.43
1:E:111:ILE:HD12	1:E:111:ILE:N	2.33	0.43
1:B:48:LEU:HD12	1:B:49:ARG:N	2.34	0.43
1:B:199:GLN:HE22	1:B:272:ARG:HH22	1.67	0.43
1:D:241:LEU:HD23	1:D:270:PHE:CE2	2.52	0.43
1:E:20:GLY:O	1:E:30:LEU:HD12	2.18	0.43
1:C:109:ASP:OD2	1:C:118:ARG:NH1	2.52	0.43
1:D:161:VAL:HG13	1:D:177:ALA:HB2	2.00	0.43
1:D:228:ILE:CD1	1:D:306:VAL:HG11	2.48	0.43
1:E:66:GLU:OE2	1:E:66:GLU:N	2.52	0.43
1:E:145:PRO:HG2	1:E:227:THR:HG23	2.00	0.43
1:D:63:PHE:HB2	1:D:103:ASN:ND2	2.23	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:MSE:HG3	1:E:334:LEU:HG	2.01	0.43
1:A:278:ARG:HD3	1:A:292:VAL:HG11	1.98	0.43
1:B:141:ARG:HD2	1:B:141:ARG:N	2.34	0.43
1:C:274:THR:HG22	1:C:277:GLU:CG	2.47	0.43
1:E:90:LEU:HD13	1:E:90:LEU:C	2.44	0.43
1:B:68:LEU:HD12	1:B:68:LEU:HA	1.92	0.43
1:C:53:LEU:HG	1:C:63:PHE:CE1	2.53	0.43
1:B:31:LYS:HE2	1:B:42:GLU:OE2	2.19	0.43
1:B:182:ILE:HD12	1:B:182:ILE:O	2.19	0.43
1:A:236:THR:HG21	1:A:325:GLU:OE1	2.19	0.43
1:A:274:THR:HG22	1:A:277:GLU:N	2.17	0.42
1:D:25:THR:HA	1:D:97:ALA:HB2	2.01	0.42
1:D:118:ARG:HG3	1:D:119:PRO:HD2	2.00	0.42
1:D:186:ARG:HG2	1:D:187:MSE:CE	2.49	0.42
1:E:53:LEU:HD22	1:E:63:PHE:CD1	2.54	0.42
1:E:143:ASP:O	1:E:144:LEU:HD22	2.19	0.42
1:C:31:LYS:HB2	1:C:329:LEU:HD13	2.02	0.42
1:C:173:GLN:NE2	1:C:175:GLN:HE22	2.07	0.42
1:D:186:ARG:HG2	1:D:187:MSE:HE2	2.01	0.42
1:A:143:ASP:C	1:A:144:LEU:HD12	2.44	0.42
1:A:144:LEU:HA	1:A:145:PRO:HD2	1.98	0.42
1:C:28:ILE:HG22	1:C:51:ILE:HD12	2.01	0.42
1:E:28:ILE:HG22	1:E:49:ARG:O	2.20	0.42
1:D:199:GLN:OE1	1:D:272:ARG:NH2	2.52	0.42
1:E:57:VAL:O	1:E:57:VAL:HG12	2.19	0.42
1:E:101:ALA:HB1	1:E:103:ASN:ND2	2.35	0.42
1:B:187:MSE:HE2	1:B:187:MSE:HA	2.02	0.42
1:D:213:ILE:HG21	1:D:305:ARG:HG3	2.02	0.42
1:E:102:GLU:C	1:E:104:ARG:H	2.27	0.42
1:A:199:GLN:HB2	1:D:145:PRO:HA	2.02	0.42
1:B:33:ALA:HA	1:B:43:VAL:HG23	2.02	0.42
1:C:285:HIS:CD2	1:C:286:PRO:HD2	2.55	0.41
1:D:321:PHE:CD1	1:D:321:PHE:C	2.98	0.41
1:A:40:MSE:HE2	1:A:334:LEU:HG	2.01	0.41
1:B:275:ARG:O	1:B:279:ARG:HG3	2.21	0.41
1:B:284:ILE:HD12	1:B:284:ILE:N	2.35	0.41
1:C:140:ASN:ND2	1:C:142:ASP:HB3	2.33	0.41
1:D:31:LYS:HB3	1:D:329:LEU:HD11	2.01	0.41
1:D:108:GLU:HA	1:D:119:PRO:HG3	2.02	0.41
1:D:258:LEU:HD23	1:D:258:LEU:HA	1.89	0.41
1:E:76:ARG:HA	1:E:114:ILE:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:VAL:HG22	1:C:291:VAL:HG11	2.03	0.41
1:D:40:MSE:HE2	1:D:334:LEU:HG	2.03	0.41
1:A:227:THR:HG22	1:A:229:ILE:CD1	2.51	0.41
1:D:58:ASP:OD2	1:D:190:ARG:HD2	2.20	0.41
1:E:149:LEU:HB2	1:E:225:ALA:HB2	2.03	0.41
1:A:53:LEU:HG	1:A:63:PHE:CE1	2.55	0.41
1:D:254:ASP:HB2	1:D:325:GLU:CG	2.50	0.41
1:C:197:PRO:CG	1:C:202:ILE:HD11	2.51	0.41
1:A:198:THR:OG1	1:A:201:GLN:HG3	2.20	0.41
1:B:91:ARG:NH2	1:B:122:ILE:HG21	2.35	0.41
1:B:122:ILE:CD1	1:B:127:GLU:HB2	2.51	0.41
1:B:143:ASP:HB2	1:B:144:LEU:HD12	2.02	0.41
1:D:138:VAL:HG21	1:D:330:ASP:HB3	2.01	0.41
1:D:215:GLU:HA	1:D:218:ARG:CZ	2.51	0.41
1:E:43:VAL:HG11	1:E:85:HIS:NE2	2.35	0.41
1:B:82:ILE:CG2	1:B:87:ILE:HD12	2.47	0.41
1:B:149:LEU:HD23	1:B:162:ILE:HB	2.02	0.41
1:D:25:THR:HG23	1:D:54:GLY:HA3	2.03	0.41
1:A:149:LEU:HB2	1:A:225:ALA:HB2	2.03	0.40
1:C:104:ARG:O	1:C:108:GLU:HG3	2.21	0.40
1:C:112:GLU:HA	1:C:117:VAL:O	2.21	0.40
1:C:246:LYS:HB2	1:C:246:LYS:NZ	2.36	0.40
1:C:257:ARG:HH11	1:C:257:ARG:CB	2.27	0.40
1:A:273:MSE:HG2	1:A:277:GLU:CB	2.51	0.40
1:B:284:ILE:HG22	1:B:289:ILE:HG13	2.04	0.40
1:E:31:LYS:HE3	1:E:42:GLU:OE2	2.21	0.40
1:E:247:GLU:HB2	1:E:248:TYR:H	1.49	0.40
1:B:298:VAL:O	1:B:302:VAL:HG23	2.21	0.40
1:D:72:TYR:CE1	1:D:110:GLU:HG2	2.56	0.40
1:D:87:ILE:H	1:D:87:ILE:CD1	2.31	0.40
1:E:62:ARG:HA	1:E:101:ALA:CB	2.50	0.40
1:E:199:GLN:HE22	1:E:272:ARG:NH1	2.19	0.40
1:E:336:TYR:HD1	1:E:339:ARG:NH2	2.19	0.40
1:A:146:ALA:HB1	1:A:147:PRO:HA	2.04	0.40
1:A:274:THR:CG2	1:A:277:GLU:HG3	2.51	0.40
1:B:126:GLU:O	1:B:130:LEU:HG	2.21	0.40
1:D:69:GLU:HA	1:D:72:TYR:CD2	2.57	0.40
1:E:54:GLY:C	1:E:57:VAL:HG23	2.47	0.40
1:A:256:HIS:HE1	3:A:374:HOH:O	2.04	0.40
1:B:133:LEU:HA	1:B:136:THR:HG22	2.03	0.40
1:D:186:ARG:O	1:D:190:ARG:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	328/343 (96%)	317 (97%)	8 (2%)	3 (1%)	14	22
1	B	328/343 (96%)	316 (96%)	10 (3%)	2 (1%)	21	32
1	C	331/343 (96%)	321 (97%)	9 (3%)	1 (0%)	36	50
1	D	328/343 (96%)	307 (94%)	18 (6%)	3 (1%)	14	22
1	E	318/343 (93%)	296 (93%)	19 (6%)	3 (1%)	14	22
All	All	1633/1715 (95%)	1557 (95%)	64 (4%)	12 (1%)	18	28

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	247	GLU
1	D	252	VAL
1	B	181	ASN
1	B	232	SER
1	C	232	SER
1	D	251	THR
1	E	108	GLU
1	E	232	SER
1	A	46	ARG
1	A	232	SER
1	A	342	ALA
1	E	138	VAL

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	264/268 (98%)	247 (94%)	17 (6%)	16	28
1	B	264/268 (98%)	254 (96%)	10 (4%)	29	49
1	C	267/268 (100%)	249 (93%)	18 (7%)	15	26
1	D	264/268 (98%)	248 (94%)	16 (6%)	17	30
1	E	258/268 (96%)	247 (96%)	11 (4%)	26	44
All	All	1317/1340 (98%)	1245 (94%)	72 (6%)	19	34

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	68	LEU
1	A	133	LEU
1	A	136	THR
1	A	159	GLU
1	A	161	VAL
1	A	190	ARG
1	A	241	LEU
1	A	258	LEU
1	A	271	LEU
1	A	274	THR
1	A	289	ILE
1	A	290	ASP
1	A	329	LEU
1	A	333	VAL
1	A	334	LEU
1	A	343	GLN
1	B	87	ILE
1	B	149	LEU
1	B	171	THR
1	B	190	ARG
1	B	194	ASN
1	B	219	THR
1	B	241	LEU
1	B	258	LEU
1	B	271	LEU
1	B	329	LEU
1	C	51	ILE

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Mol	Chain	Res	Type
1	C	68	LEU
1	C	87	ILE
1	C	122	ILE
1	C	133	LEU
1	C	136	THR
1	C	141	ARG
1	C	142	ASP
1	C	149	LEU
1	C	161	VAL
1	C	219	THR
1	C	241	LEU
1	C	246	LYS
1	C	257	ARG
1	C	271	LEU
1	C	274	THR
1	C	329	LEU
1	C	333	VAL
1	D	51	ILE
1	D	59	LYS
1	D	87	ILE
1	D	133	LEU
1	D	139	VAL
1	D	142	ASP
1	D	159	GLU
1	D	161	VAL
1	D	182	ILE
1	D	219	THR
1	D	250	HIS
1	D	258	LEU
1	D	271	LEU
1	D	272	ARG
1	D	334	LEU
1	D	340	LEU
1	E	53	LEU
1	E	68	LEU
1	E	103	ASN
1	E	122	ILE
1	E	159	GLU
1	E	161	VAL
1	E	226	ARG
1	E	247	GLU
1	E	258	LEU

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Mol	Chain	Res	Type
1	E	271	LEU
1	E	334	LEU

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	26	ASN
1	A	175	GLN
1	A	256	HIS
1	A	285	HIS
1	A	314	HIS
1	A	326	HIS
1	A	343	GLN
1	B	85	HIS
1	B	140	ASN
1	B	175	GLN
1	B	181	ASN
1	B	194	ASN
1	B	199	GLN
1	B	314	HIS
1	C	140	ASN
1	C	173	GLN
1	C	199	GLN
1	C	285	HIS
1	C	314	HIS
1	C	326	HIS
1	D	85	HIS
1	D	173	GLN
1	D	314	HIS
1	E	103	ASN
1	E	140	ASN
1	E	191	HIS
1	E	194	ASN
1	E	199	GLN
1	E	201	GLN
1	E	212	HIS
1	E	314	HIS

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](#)

16 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	SO4	B	344	-	4,4,4	0.37	0	6,6,6	0.10	0
2	SO4	D	344	-	4,4,4	0.36	0	6,6,6	0.08	0
2	SO4	B	346	-	4,4,4	0.39	0	6,6,6	0.08	0
2	SO4	A	344	-	4,4,4	0.34	0	6,6,6	0.19	0
2	SO4	C	344	-	4,4,4	0.45	0	6,6,6	0.12	0
2	SO4	A	346	-	4,4,4	0.43	0	6,6,6	0.22	0
2	SO4	C	346	-	4,4,4	0.37	0	6,6,6	0.13	0
2	SO4	D	346	-	4,4,4	0.37	0	6,6,6	0.07	0
2	SO4	E	345	-	4,4,4	0.35	0	6,6,6	0.08	0
2	SO4	C	345	-	4,4,4	0.42	0	6,6,6	0.14	0
2	SO4	E	344	-	4,4,4	0.38	0	6,6,6	0.08	0
2	SO4	B	345	-	4,4,4	0.38	0	6,6,6	0.24	0
2	SO4	A	345	-	4,4,4	0.35	0	6,6,6	0.18	0
2	SO4	E	346	-	4,4,4	0.39	0	6,6,6	0.09	0
2	SO4	D	345	-	4,4,4	0.36	0	6,6,6	0.08	0
2	SO4	C	347	-	4,4,4	0.41	0	6,6,6	0.19	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	346	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, 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	324/343 (94%)	-0.08	2 (0%) 85 83	14, 29, 56, 81	0
1	B	324/343 (94%)	0.53	19 (5%) 28 24	22, 43, 74, 85	0
1	C	326/343 (95%)	-0.24	7 (2%) 63 59	10, 24, 57, 87	0
1	D	324/343 (94%)	0.88	36 (11%) 10 7	19, 56, 79, 93	0
1	E	316/343 (92%)	1.25	74 (23%) 2 1	33, 61, 93, 100	0
All	All	1614/1715 (94%)	0.46	138 (8%) 16 13	10, 43, 82, 100	0

All (138) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	39	GLY	6.7
1	E	115	LEU	5.8
1	D	142	ASP	4.9
1	E	117	VAL	4.8
1	E	248	TYR	4.8
1	E	83	ALA	4.5
1	E	87	ILE	4.1
1	E	60	THR	3.9
1	B	248	TYR	3.8
1	E	79	ALA	3.8
1	C	250	HIS	3.7
1	D	276	ALA	3.7
1	B	138	VAL	3.7
1	E	97	ALA	3.6
1	B	100	ASP	3.6
1	D	248	TYR	3.6
1	E	341	LEU	3.5
1	E	78	PHE	3.5
1	D	249	ASP	3.5
1	E	17	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	251	THR	3.5
1	C	142	ASP	3.4
1	D	64	ALA	3.4
1	C	12	SER	3.4
1	E	22	ASP	3.4
1	D	250	HIS	3.3
1	D	111	ILE	3.3
1	E	63	PHE	3.2
1	D	251	THR	3.2
1	E	123	PRO	3.2
1	E	45	PRO	3.1
1	E	43	VAL	3.1
1	B	98	THR	3.1
1	E	247	GLU	3.1
1	E	138	VAL	3.1
1	E	125	THR	3.0
1	A	342	ALA	3.0
1	E	100	ASP	3.0
1	E	80	GLY	3.0
1	E	16	VAL	2.9
1	E	53	LEU	2.9
1	D	107	PHE	2.9
1	D	96	SER	2.9
1	D	73	VAL	2.9
1	E	111	ILE	2.9
1	D	139	VAL	2.9
1	E	128	ALA	2.9
1	E	107	PHE	2.9
1	E	287	GLY	2.9
1	E	114	ILE	2.8
1	B	249	ASP	2.8
1	E	246	LYS	2.8
1	D	97	ALA	2.8
1	D	13	LYS	2.8
1	B	289	ILE	2.8
1	D	198	THR	2.8
1	E	139	VAL	2.7
1	E	98	THR	2.7
1	E	124	GLY	2.7
1	E	101	ALA	2.7
1	E	26	ASN	2.7
1	C	248	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	283	THR	2.7
1	E	339	ARG	2.7
1	B	342	ALA	2.7
1	D	342	ALA	2.7
1	E	333	VAL	2.6
1	B	97	ALA	2.6
1	E	88	ASP	2.6
1	C	141	ARG	2.6
1	E	66	GLU	2.6
1	B	37	ALA	2.6
1	D	136	THR	2.6
1	E	67	ALA	2.6
1	E	69	GLU	2.5
1	E	50	VAL	2.5
1	E	64	ALA	2.5
1	E	85	HIS	2.5
1	E	89	GLY	2.5
1	E	21	ILE	2.5
1	E	58	ASP	2.5
1	E	81	VAL	2.5
1	D	79	ALA	2.5
1	C	251	THR	2.5
1	B	39	GLY	2.4
1	E	116	GLY	2.4
1	E	143	ASP	2.4
1	D	138	VAL	2.4
1	E	48	LEU	2.4
1	E	112	GLU	2.4
1	B	340	LEU	2.3
1	D	65	ASP	2.3
1	E	252	VAL	2.3
1	E	113	ARG	2.3
1	D	114	ILE	2.3
1	E	109	ASP	2.3
1	E	18	VAL	2.3
1	D	63	PHE	2.3
1	D	252	VAL	2.3
1	E	62	ARG	2.3
1	E	47	ILE	2.2
1	C	249	ASP	2.2
1	D	69	GLU	2.2
1	E	325	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	93	VAL	2.2
1	B	124	GLY	2.2
1	E	94	ALA	2.2
1	E	41	HIS	2.2
1	D	157	SER	2.2
1	E	290	ASP	2.2
1	E	102	GLU	2.2
1	B	291	VAL	2.2
1	D	74	ALA	2.2
1	B	136	THR	2.2
1	D	245	LEU	2.2
1	B	26	ASN	2.1
1	B	38	ASP	2.1
1	E	86	PRO	2.1
1	B	250	HIS	2.1
1	D	193	THR	2.1
1	E	25	THR	2.1
1	D	284	ILE	2.1
1	D	52	ARG	2.1
1	D	113	ARG	2.1
1	E	136	THR	2.1
1	D	291	VAL	2.1
1	E	334	LEU	2.1
1	D	67	ALA	2.0
1	A	340	LEU	2.0
1	D	140	ASN	2.0
1	B	333	VAL	2.0
1	E	44	VAL	2.0
1	E	46	ARG	2.0
1	E	57	VAL	2.0
1	E	121	VAL	2.0
1	E	340	LEU	2.0
1	D	246	LYS	2.0
1	D	290	ASP	2.0

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

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
2	SO4	E	345	5/5	0.66	0.21	117,117,118,118	0
2	SO4	B	346	5/5	0.72	0.20	91,92,93,93	0
2	SO4	A	346	5/5	0.72	0.26	58,59,63,65	0
2	SO4	E	346	5/5	0.72	0.23	98,98,98,99	0
2	SO4	C	347	5/5	0.74	0.23	67,68,69,72	0
2	SO4	E	344	5/5	0.75	0.17	85,85,86,86	0
2	SO4	D	346	5/5	0.79	0.19	90,91,91,92	0
2	SO4	D	344	5/5	0.80	0.19	81,83,83,84	0
2	SO4	B	345	5/5	0.84	0.16	59,60,60,62	0
2	SO4	C	346	5/5	0.86	0.21	74,74,75,77	0
2	SO4	C	345	5/5	0.91	0.16	59,59,61,63	0
2	SO4	B	344	5/5	0.93	0.11	56,57,58,59	0
2	SO4	D	345	5/5	0.93	0.10	55,55,56,57	0
2	SO4	A	345	5/5	0.93	0.14	52,53,54,55	0
2	SO4	C	344	5/5	0.98	0.06	29,30,31,32	0
2	SO4	A	344	5/5	0.98	0.07	31,31,32,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.