



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:35 AM UTC

PDB ID : 1Z5H / pdb_00001z5h
Title : Crystal structures of the Tricorn interacting Factor F3 from *Thermoplasma acidophilum*
Authors : Kyrieleis, O.J.P.; Goettig, P.; Kiefersauer, R.; Huber, R.; Brandstetter, H.
Deposited on : 2005-03-18
Resolution : 2.30 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

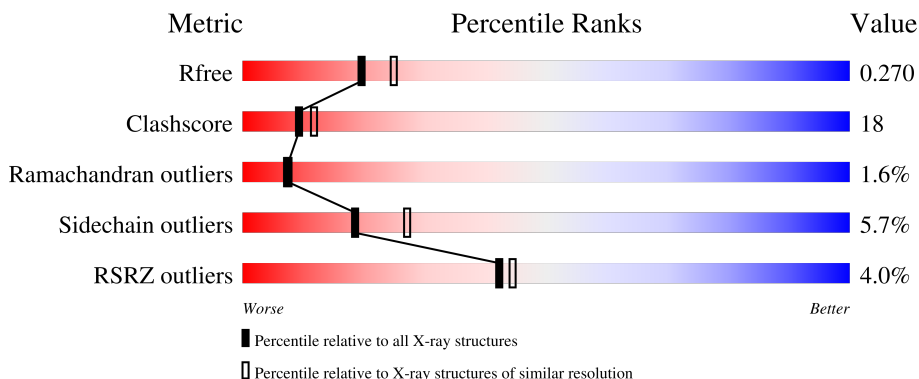
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	780	3% 66% 31% .
1	B	780	5% 62% 32% 5%

2 Entry composition [i](#)

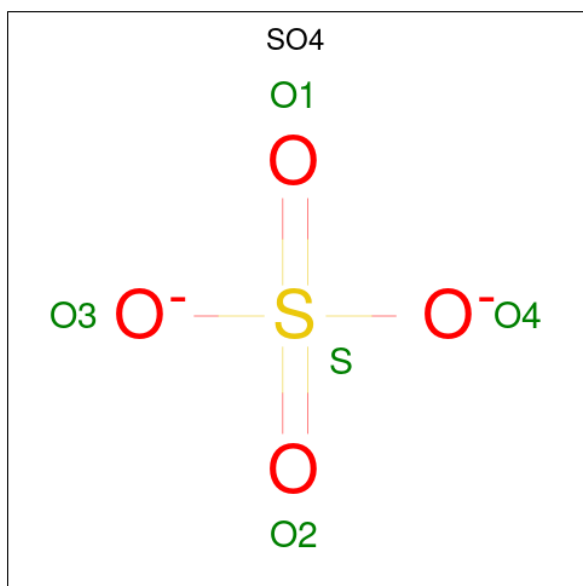
There are 4 unique types of molecules in this entry. The entry contains 13456 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Tricorn protease interacting factor F3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	780	Total	C	N	O	S	2	0	0
			6295	4008	1066	1190	31			
1	B	780	Total	C	N	O	S	8	0	0
			6295	4008	1066	1190	31			

- 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	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0

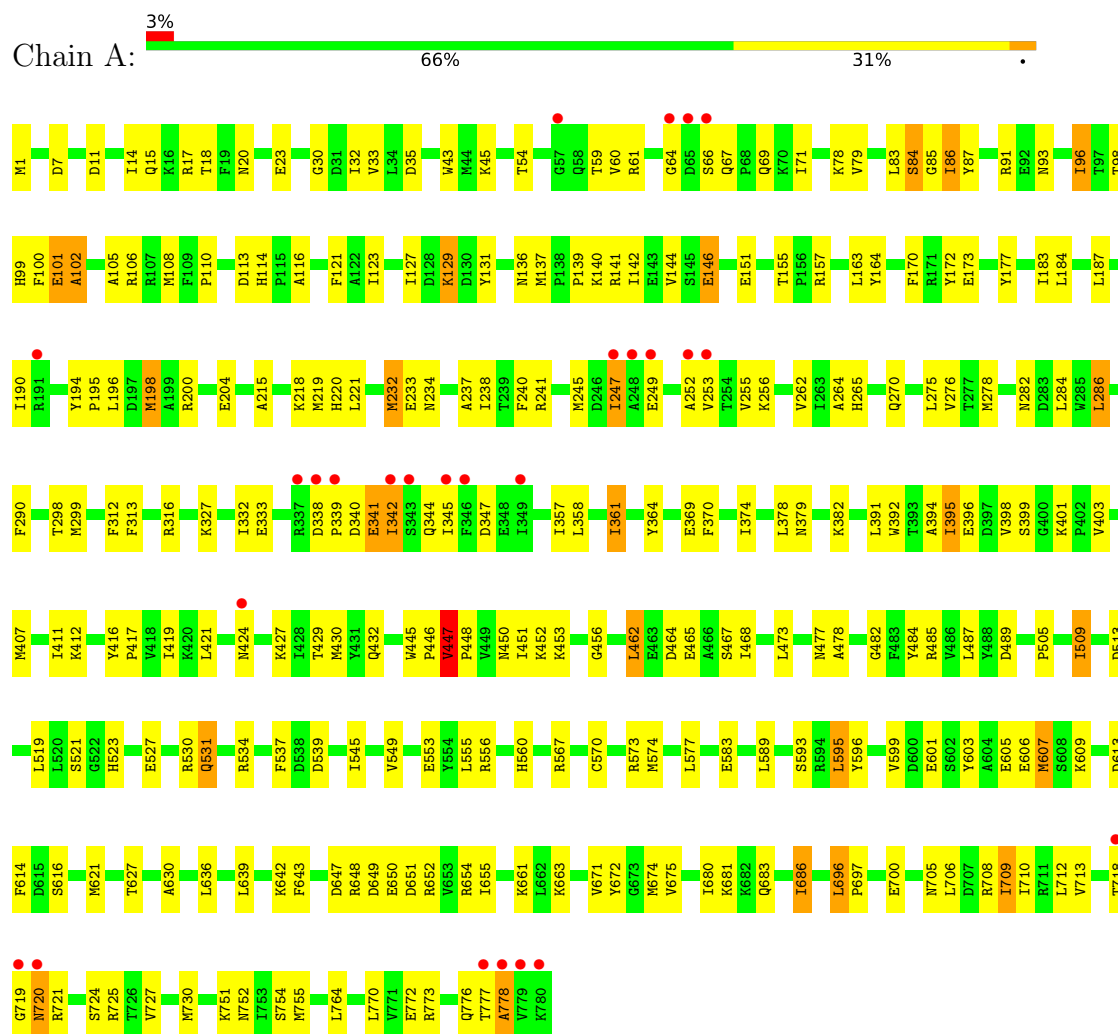
- Molecule 4 is water.

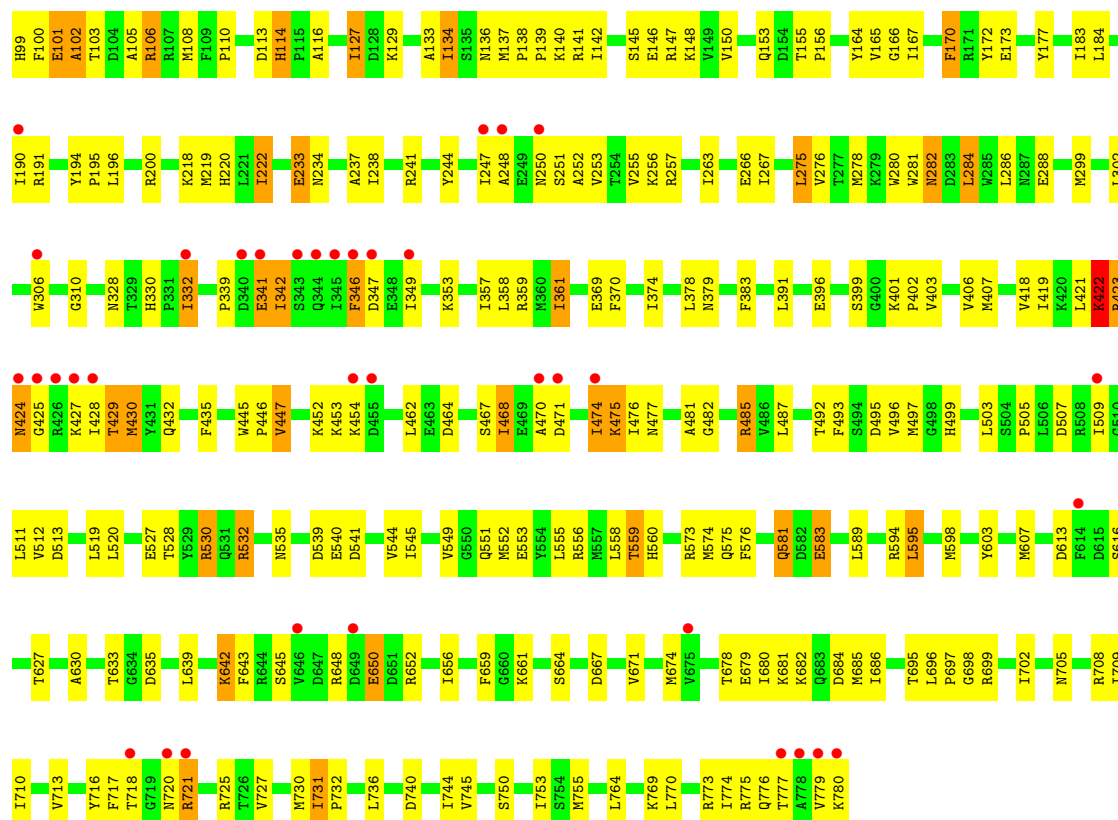
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	442	Total O 442 442	0	0
4	B	337	Total O 337 337	0	0

3 Residue-property plots

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: Tricorn protease interacting factor F3





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	115.20Å 183.30Å 105.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.48 – 2.30 19.48 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.48-2.30) 99.7 (19.48-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.04 (at 2.30Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.225 , 0.270 0.225 , 0.270	Depositor DCC
R_{free} test set	5029 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13456	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.19% 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, ZN

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	0/6429	0.90	12/8677 (0.1%)
1	B	0.45	0/6429	0.90	19/8677 (0.2%)
All	All	0.46	0/12858	0.90	31/17354 (0.2%)

There are no bond length outliers.

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	447	VAL	N-CA-C	9.63	117.49	107.76
1	A	447	VAL	N-CA-C	9.02	117.87	107.77
1	B	96	ILE	N-CA-C	-7.26	99.33	109.21
1	A	446	PRO	N-CA-C	-7.21	97.62	112.47
1	A	96	ILE	N-CA-C	-6.76	100.02	109.21
1	A	730	MET	N-CA-C	6.55	118.21	111.14
1	B	310	GLY	N-CA-C	-6.36	104.80	112.49
1	A	489	ASP	N-CA-C	-6.34	102.34	110.53
1	B	730	MET	N-CA-C	6.32	117.97	111.14
1	B	146	GLU	N-CA-C	-6.30	104.65	112.90
1	A	241	ARG	N-CA-C	-6.05	101.32	110.28
1	B	370	PHE	N-CA-C	-5.97	104.69	111.14
1	B	222	ILE	N-CA-C	5.89	116.59	107.99
1	B	446	PRO	N-CA-C	-5.86	100.40	112.47
1	B	170	PHE	N-CA-C	5.79	118.66	110.50
1	A	146	GLU	N-CA-C	-5.76	104.97	112.23
1	A	215	ALA	N-CA-C	5.74	119.55	112.54
1	B	172	TYR	N-CA-C	5.55	118.12	109.52
1	A	105	ALA	N-CA-C	-5.53	105.34	111.71
1	B	731	ILE	CB-CA-C	-5.48	108.50	113.70
1	A	170	PHE	N-CA-C	5.41	117.67	110.53
1	B	156	PRO	N-CA-C	-5.39	101.36	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	140	LYS	N-CA-C	-5.31	106.49	113.12
1	B	233	GLU	N-CA-C	5.29	122.07	110.80
1	A	172	TYR	N-CA-C	5.24	117.64	109.52
1	B	8	LEU	N-CA-C	5.21	117.46	109.07
1	B	14	ILE	N-CA-C	5.18	115.90	110.62
1	B	114	HIS	CA-C-N	5.06	124.85	119.28
1	B	114	HIS	C-N-CA	5.06	124.85	119.28
1	B	447	VAL	CA-C-N	5.06	126.45	120.23
1	B	447	VAL	C-N-CA	5.06	126.45	120.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6295	0	6206	208	0
1	B	6295	0	6206	246	0
2	A	65	0	0	3	0
2	B	20	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	442	0	0	24	0
4	B	337	0	0	9	0
All	All	13456	0	12412	454	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 18.

All (454) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ILE:HD13	4:B:2040:HOH:O	1.50	1.09
1:B:332:ILE:HD11	1:B:353:LYS:HD3	1.34	1.09
1:A:357:ILE:HD13	1:A:407:MET:HE1	1.15	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ARG:HH21	1:A:113:ASP:HB3	1.20	1.02
1:A:233:GLU:HA	1:A:238:ILE:HD12	1.37	1.01
1:B:142:ILE:HD12	1:B:150:VAL:HG22	1.36	1.01
1:B:133:ALA:C	1:B:134:ILE:HD12	1.84	1.01
1:A:477:ASN:HD21	1:A:482:GLY:H	1.09	0.96
1:A:391:LEU:O	1:A:395:ILE:HD13	1.67	0.95
1:A:451:ILE:HD13	1:A:468:ILE:HD13	1.50	0.93
1:A:705:ASN:O	1:A:709:ILE:HD13	1.68	0.93
1:B:40:GLN:HE21	1:B:42:ASN:HD21	1.15	0.92
1:A:357:ILE:CD1	1:A:407:MET:HE1	2.01	0.90
1:B:477:ASN:HD21	1:B:482:GLY:H	1.19	0.90
1:A:357:ILE:HD12	1:A:358:LEU:N	1.88	0.89
1:A:545:ILE:HD12	1:A:573:ARG:HG3	1.56	0.87
1:B:686:ILE:HG21	1:B:725:ARG:HH12	1.40	0.85
1:B:114:HIS:HD2	1:B:116:ALA:H	1.25	0.85
1:B:134:ILE:HD13	1:B:170:PHE:CE2	2.14	0.82
1:A:238:ILE:HD11	1:A:270:GLN:NE2	1.95	0.80
1:A:14:ILE:HD12	1:A:14:ILE:H	1.45	0.80
1:A:539:ASP:O	1:A:545:ILE:HD11	1.81	0.80
1:B:497:MET:HE2	1:B:535:ASN:HB3	1.64	0.79
1:B:423:ARG:HG2	1:B:428:ILE:HG12	1.65	0.79
1:B:432:GLN:HE22	1:B:445:TRP:H	1.31	0.78
1:A:121:PHE:HB3	1:A:123:ILE:HD11	1.66	0.78
1:B:474:ILE:HD13	1:B:474:ILE:O	1.82	0.77
1:B:103:THR:O	1:B:106:ARG:HD3	1.84	0.77
1:A:234:ASN:HB2	1:A:237:ALA:O	1.83	0.77
1:B:396:GLU:HG3	1:B:401:LYS:O	1.85	0.77
1:A:537:PHE:O	1:A:573:ARG:HD3	1.85	0.76
1:A:432:GLN:HE22	1:A:445:TRP:H	1.33	0.75
1:B:497:MET:HE2	1:B:535:ASN:CB	2.15	0.75
1:A:106:ARG:NH2	1:A:113:ASP:HB3	2.00	0.74
1:A:249:GLU:HA	1:A:256:LYS:HD3	1.69	0.74
1:B:361:ILE:HD13	1:B:361:ILE:O	1.88	0.74
1:A:396:GLU:HG3	1:A:401:LYS:O	1.89	0.73
1:B:627:THR:HG23	1:B:661:LYS:HG2	1.71	0.73
1:A:567:ARG:HD3	4:A:2331:HOH:O	1.89	0.72
1:B:1:MET:HE2	1:B:34:LEU:HD21	1.71	0.72
1:A:177:TYR:HB2	1:A:200:ARG:HG3	1.72	0.72
1:B:447:VAL:HG13	1:B:462:LEU:HB3	1.72	0.72
1:A:114:HIS:HD2	1:A:116:ALA:H	1.37	0.71
1:A:195:PRO:HD3	1:A:247:ILE:HD11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:GLU:OE1	1:B:110:PRO:HG2	1.90	0.71
1:A:238:ILE:HD11	1:A:270:GLN:HE22	1.54	0.71
1:A:86:ILE:HG13	1:A:108:MET:HE3	1.73	0.70
1:A:357:ILE:HD13	1:A:407:MET:CE	2.08	0.70
1:B:69:GLN:HG3	1:B:71:ILE:HD11	1.73	0.70
1:A:573:ARG:HD2	1:A:573:ARG:N	2.05	0.70
1:B:32:ILE:HD11	1:B:64:GLY:CA	2.23	0.69
1:A:218:LYS:NZ	1:A:220:HIS:HD2	1.90	0.69
1:B:705:ASN:HD22	1:B:708:ARG:HD2	1.57	0.69
1:A:772:GLU:HG3	1:A:776:GLN:HE21	1.58	0.69
1:B:191:ARG:HH21	1:B:248:ALA:HB2	1.58	0.69
1:B:674:MET:HB3	1:B:680:ILE:HD13	1.75	0.68
1:A:627:THR:HG23	1:A:661:LYS:HG3	1.74	0.68
1:B:263:ILE:O	1:B:267:ILE:HG12	1.94	0.68
1:B:219:MET:SD	1:B:267:ILE:HD12	2.33	0.68
1:B:252:ALA:O	1:B:255:VAL:HG22	1.93	0.68
1:A:93:ASN:HB3	4:A:2318:HOH:O	1.94	0.67
1:A:754:SER:HB2	4:A:2214:HOH:O	1.92	0.67
1:B:32:ILE:HD11	1:B:64:GLY:HA3	1.76	0.67
1:B:238:ILE:HD12	1:B:238:ILE:H	1.59	0.67
1:A:374:ILE:HD13	1:A:391:LEU:HD11	1.75	0.67
1:A:630:ALA:HB2	1:A:639:LEU:HD11	1.76	0.67
1:A:264:ALA:HB2	1:A:299:MET:HE3	1.76	0.66
1:B:40:GLN:HE21	1:B:42:ASN:ND2	1.91	0.66
1:B:559:THR:HG21	1:B:774:ILE:HD13	1.76	0.66
1:B:359:ARG:NH2	1:B:481:ALA:HA	2.10	0.66
1:A:247:ILE:HD13	1:A:247:ILE:H	1.60	0.66
1:A:341:GLU:HB2	1:A:345:ILE:HG22	1.78	0.66
1:A:450:ASN:HD21	1:A:478:ALA:HB3	1.60	0.66
1:B:452:LYS:HE3	1:B:474:ILE:HD12	1.77	0.65
1:A:139:PRO:HB2	1:A:142:ILE:HD11	1.78	0.65
1:A:452:LYS:HE3	1:A:478:ALA:HB1	1.76	0.65
1:A:485:ARG:NH1	1:A:513:ASP:OD1	2.29	0.65
1:B:705:ASN:O	1:B:709:ILE:HD13	1.97	0.65
1:B:342:ILE:HD11	1:B:721:ARG:HH12	1.61	0.65
1:B:136:ASN:HD21	1:B:164:TYR:H	1.43	0.65
1:B:552:MET:HB2	1:B:595:LEU:HD11	1.78	0.64
1:B:133:ALA:O	1:B:134:ILE:HD12	1.97	0.64
1:B:141:ARG:O	1:B:142:ILE:HD13	1.98	0.63
1:B:184:LEU:HD22	1:B:190:ILE:CD1	2.28	0.63
1:B:633:THR:CG2	1:B:635:ASP:HB2	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:ILE:CD1	1:B:150:VAL:HG13	2.29	0.63
1:B:432:GLN:NE2	1:B:445:TRP:H	1.96	0.63
1:B:541:ASP:O	1:B:545:ILE:HG12	1.99	0.62
1:B:88:TYR:HD1	1:B:96:ILE:HD13	1.64	0.62
1:B:731:ILE:HD11	1:B:745:VAL:HG21	1.82	0.62
1:A:419:ILE:HD13	1:A:484:TYR:CD1	2.35	0.62
1:A:369:GLU:HG2	4:A:2367:HOH:O	2.00	0.62
1:A:69:GLN:CD	1:A:71:ILE:HD11	2.24	0.61
1:A:342:ILE:HD13	1:A:342:ILE:O	2.00	0.61
1:B:184:LEU:HD22	1:B:190:ILE:HD13	1.82	0.61
1:B:422:LYS:HG3	1:B:429:THR:HG23	1.81	0.61
1:A:278:MET:HE2	4:A:2078:HOH:O	2.00	0.61
1:B:633:THR:HG22	1:B:635:ASP:HB2	1.82	0.61
1:A:509:ILE:HB	4:A:2267:HOH:O	2.01	0.61
1:B:428:ILE:HD12	1:B:470:ALA:HA	1.83	0.61
1:A:447:VAL:HG13	1:A:462:LEU:HB3	1.83	0.61
1:B:581:GLN:CD	1:B:581:GLN:H	2.08	0.61
1:A:451:ILE:CD1	1:A:468:ILE:HD13	2.28	0.60
1:A:773:ARG:O	1:A:777:THR:HG22	2.01	0.60
1:B:539:ASP:O	1:B:545:ILE:HD11	2.00	0.60
1:A:253:VAL:HG23	4:A:2158:HOH:O	2.02	0.60
1:A:139:PRO:CB	1:A:142:ILE:HD11	2.32	0.60
1:B:114:HIS:CD2	1:B:116:ALA:H	2.15	0.60
1:A:357:ILE:HD12	1:A:357:ILE:C	2.27	0.59
1:A:601:GLU:O	1:A:605:GLU:HG3	2.02	0.59
1:B:674:MET:CB	1:B:680:ILE:HD13	2.32	0.59
1:A:549:VAL:O	1:A:553:GLU:HG3	2.02	0.59
1:A:341:GLU:HB2	1:A:345:ILE:H	1.67	0.59
1:A:708:ARG:HB3	4:A:2213:HOH:O	2.02	0.59
1:B:139:PRO:HB3	1:B:142:ILE:HD11	1.85	0.59
1:B:137:MET:HG2	1:B:155:THR:HG22	1.85	0.59
1:A:141:ARG:C	1:A:142:ILE:HD12	2.28	0.58
1:A:234:ASN:O	1:A:238:ILE:HD13	2.03	0.58
1:B:369:GLU:OE2	1:B:399:SER:HA	2.03	0.58
1:B:106:ARG:HD2	1:B:113:ASP:OD2	2.03	0.58
1:B:528:THR:O	1:B:532:ARG:HG3	2.03	0.58
1:A:101:GLU:O	1:A:102:ALA:CB	2.52	0.58
1:A:196:LEU:HD23	1:A:221:LEU:HD12	1.86	0.58
1:A:23:GLU:OE1	1:A:110:PRO:HG2	2.04	0.57
1:A:157:ARG:HD3	4:A:2189:HOH:O	2.03	0.57
1:B:253:VAL:O	1:B:257:ARG:HG2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:GLN:NE2	1:A:445:TRP:H	2.01	0.57
1:B:100:PHE:O	1:B:101:GLU:C	2.46	0.57
1:A:672:TYR:CZ	1:A:709:ILE:HD12	2.39	0.57
1:B:257:ARG:HG3	1:B:306:TRP:CZ2	2.39	0.57
1:A:643:PHE:CZ	1:A:680:ILE:HD13	2.38	0.57
1:B:779:VAL:O	1:B:780:LYS:HG3	2.04	0.57
1:A:671:VAL:HA	1:A:674:MET:HE2	1.86	0.57
1:A:614:PHE:HB3	1:A:642:LYS:HE2	1.86	0.57
1:B:474:ILE:HD13	1:B:474:ILE:C	2.29	0.57
1:A:312:PHE:O	1:A:316:ARG:HB2	2.04	0.57
1:B:710:ILE:CD1	1:B:745:VAL:HG22	2.35	0.56
1:A:613:ASP:HB3	1:A:616:SER:HB3	1.88	0.56
1:B:166:GLY:C	1:B:167:ILE:HD12	2.31	0.56
1:B:251:SER:O	1:B:256:LYS:HE3	2.06	0.56
1:B:652:ARG:O	1:B:656:ILE:HG12	2.06	0.56
1:B:452:LYS:CE	1:B:474:ILE:HD12	2.35	0.56
1:B:574:MET:HE1	1:B:589:LEU:HD12	1.88	0.55
1:A:686:ILE:HB	4:A:2249:HOH:O	2.05	0.55
1:A:755:MET:HB2	4:A:2392:HOH:O	2.06	0.55
1:B:238:ILE:HD12	1:B:238:ILE:N	2.21	0.55
1:B:101:GLU:O	1:B:102:ALA:CB	2.53	0.55
1:A:86:ILE:CG1	1:A:108:MET:HE3	2.35	0.55
1:B:177:TYR:HB2	1:B:200:ARG:HG3	1.89	0.55
1:B:454:LYS:HE3	1:B:499:HIS:CD2	2.41	0.55
1:B:95:MET:HE2	1:B:97:THR:CG2	2.37	0.55
1:B:432:GLN:HE22	1:B:445:TRP:HB2	1.72	0.55
1:B:512:VAL:HG13	1:B:551:GLN:HE22	1.72	0.55
1:A:361:ILE:CD1	1:A:403:VAL:HG13	2.36	0.55
1:B:779:VAL:HA	4:B:2252:HOH:O	2.06	0.55
1:B:218:LYS:HD2	1:B:218:LYS:C	2.33	0.54
1:B:233:GLU:O	1:B:234:ASN:C	2.50	0.54
1:B:474:ILE:O	1:B:474:ILE:CD1	2.54	0.54
1:B:682:LYS:HD2	1:B:716:TYR:O	2.08	0.54
1:A:570:CYS:O	1:A:574:MET:HB2	2.08	0.54
1:B:133:ALA:C	1:B:134:ILE:CD1	2.73	0.54
1:A:341:GLU:HB3	1:A:344:GLN:HB3	1.89	0.54
1:B:505:PRO:HG2	4:B:2014:HOH:O	2.07	0.54
1:B:32:ILE:CD1	1:B:64:GLY:CA	2.85	0.54
1:A:183:ILE:HD12	1:A:183:ILE:N	2.23	0.53
1:A:333:GLU:HB2	1:A:411:ILE:HG22	1.89	0.53
1:B:452:LYS:CD	1:B:474:ILE:HD12	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ILE:HD12	1:B:32:ILE:N	2.22	0.53
1:B:244:TYR:O	1:B:247:ILE:HD11	2.08	0.53
1:B:419:ILE:HD12	1:B:462:LEU:HD13	1.90	0.53
1:B:358:LEU:O	1:B:361:ILE:HG22	2.08	0.53
1:B:507:ASP:O	1:B:511:LEU:HG	2.09	0.53
1:B:685:MET:CE	1:B:713:VAL:HG22	2.39	0.53
1:A:333:GLU:OE2	1:A:412:LYS:HG2	2.09	0.53
1:A:560:HIS:HB2	2:A:1005:SO4:O1	2.08	0.53
1:B:485:ARG:NH1	1:B:513:ASP:OD1	2.42	0.53
1:A:651:ASP:HA	1:A:654:ARG:HD2	1.91	0.53
1:A:379:ASN:O	1:A:382:LYS:HG2	2.09	0.53
1:A:527:GLU:HG2	1:A:531:GLN:HE22	1.73	0.53
1:A:606:GLU:O	1:A:609:LYS:HG2	2.09	0.53
1:B:418:VAL:HB	1:B:435:PHE:HB2	1.90	0.53
1:A:233:GLU:CA	1:A:238:ILE:HD12	2.24	0.53
1:A:395:ILE:N	1:A:395:ILE:CD1	2.72	0.53
1:B:183:ILE:N	1:B:183:ILE:HD12	2.23	0.53
1:A:194:TYR:N	1:A:195:PRO:HD2	2.23	0.53
1:A:195:PRO:HD3	1:A:247:ILE:CD1	2.38	0.53
1:B:103:THR:HB	1:B:106:ARG:NH1	2.24	0.53
1:A:361:ILE:HG13	1:A:407:MET:SD	2.48	0.52
1:B:520:LEU:HD23	1:B:770:LEU:HD22	1.91	0.52
1:A:338:ASP:O	1:A:340:ASP:N	2.42	0.52
1:B:136:ASN:ND2	1:B:164:TYR:H	2.08	0.52
1:B:630:ALA:HB2	1:B:639:LEU:HD11	1.90	0.52
1:B:234:ASN:HB2	1:B:237:ALA:O	2.09	0.52
1:B:497:MET:CE	1:B:535:ASN:HB3	2.36	0.52
1:B:453:LYS:HA	1:B:474:ILE:HG22	1.92	0.52
1:B:492:THR:O	1:B:496:VAL:HG23	2.09	0.52
1:A:643:PHE:HB2	1:A:655:ILE:HG21	1.90	0.52
1:A:672:TYR:OH	1:A:709:ILE:HD12	2.09	0.52
1:B:328:ASN:HB3	1:B:755:MET:CE	2.40	0.52
1:A:136:ASN:HD21	1:A:164:TYR:H	1.57	0.52
1:A:607:MET:CE	1:A:621:MET:HE3	2.38	0.52
1:B:686:ILE:HG21	1:B:725:ARG:NH1	2.17	0.52
1:A:429:THR:HG22	1:A:467:SER:OG	2.10	0.52
1:B:696:LEU:N	1:B:697:PRO:HD2	2.25	0.52
1:A:709:ILE:CD1	1:A:709:ILE:N	2.72	0.52
1:B:374:ILE:HD13	1:B:391:LEU:HD11	1.91	0.52
1:B:101:GLU:O	1:B:102:ALA:HB3	2.10	0.51
1:A:364:TYR:CD1	1:A:448:PRO:HB3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:613:ASP:HB3	1:B:616:SER:OG	2.11	0.51
1:A:574:MET:HE2	1:A:603:TYR:OH	2.10	0.51
1:B:145:SER:HB2	4:B:2065:HOH:O	2.10	0.51
1:A:17:ARG:HB3	1:A:79:VAL:HB	1.91	0.51
1:A:114:HIS:CD2	1:A:116:ALA:H	2.25	0.51
1:A:69:GLN:NE2	1:A:71:ILE:HD11	2.26	0.51
1:A:252:ALA:HB3	1:A:255:VAL:HG23	1.93	0.51
1:A:361:ILE:HD12	1:A:403:VAL:HG13	1.92	0.51
1:B:142:ILE:HD11	1:B:150:VAL:HG13	1.92	0.51
1:A:341:GLU:CB	1:A:344:GLN:HB3	2.41	0.51
1:A:777:THR:HG23	4:A:2359:HOH:O	2.09	0.51
1:A:30:GLY:O	1:A:64:GLY:HA3	2.12	0.50
1:A:721:ARG:O	1:A:725:ARG:HG3	2.11	0.50
1:B:736:LEU:HD23	4:B:2218:HOH:O	2.11	0.50
1:B:421:LEU:HD23	1:B:430:MET:HB3	1.93	0.50
1:A:650:GLU:HB2	2:A:1017:SO4:O3	2.12	0.50
1:B:695:THR:O	1:B:699:ARG:HG3	2.11	0.50
1:A:706:LEU:HD11	1:A:710:ILE:HD11	1.94	0.50
1:A:100:PHE:O	1:A:101:GLU:C	2.55	0.50
1:A:136:ASN:HD21	1:A:163:LEU:HA	1.77	0.50
1:B:129:LYS:HA	1:B:148:LYS:HB2	1.94	0.50
1:A:198:MET:HE3	1:A:198:MET:HA	1.93	0.49
1:A:218:LYS:HZ2	1:A:220:HIS:HD2	1.60	0.49
1:A:432:GLN:HE22	1:A:445:TRP:HB2	1.76	0.49
1:A:15:GLN:CD	1:A:15:GLN:H	2.20	0.49
1:B:13:ASP:OD1	1:B:16:LYS:HD2	2.13	0.49
1:A:99:HIS:CE1	1:A:232:MET:HG2	2.47	0.49
1:B:95:MET:HE2	1:B:97:THR:HG21	1.93	0.49
1:A:66:SER:O	1:A:67:GLN:HB2	2.13	0.49
1:A:465:GLU:HG3	4:A:2074:HOH:O	2.13	0.49
1:B:493:PHE:CD2	1:B:532:ARG:HD2	2.47	0.49
1:B:341:GLU:O	1:B:342:ILE:HB	2.13	0.49
1:B:346:PHE:CE2	1:B:721:ARG:HD3	2.47	0.49
1:A:60:VAL:O	1:A:60:VAL:HG13	2.12	0.49
1:A:394:ALA:O	1:A:398:VAL:HG23	2.12	0.49
1:B:430:MET:HE3	1:B:462:LEU:HD12	1.95	0.49
1:B:452:LYS:HG2	1:B:474:ILE:HG23	1.94	0.49
1:B:549:VAL:O	1:B:553:GLU:HG3	2.13	0.49
1:B:750:SER:O	1:B:753:ILE:HG13	2.13	0.49
1:B:664:SER:HB3	1:B:667:ASP:OD2	2.12	0.49
1:A:607:MET:HE1	1:A:621:MET:HE3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ILE:O	1:B:61:ARG:HA	2.12	0.48
1:A:35:ASP:O	1:A:110:PRO:HA	2.14	0.48
1:A:464:ASP:O	1:A:465:GLU:C	2.56	0.48
1:A:477:ASN:ND2	1:A:482:GLY:H	1.93	0.48
1:A:613:ASP:HB2	4:A:2435:HOH:O	2.13	0.48
1:B:191:ARG:HD3	1:B:248:ALA:HB2	1.95	0.48
1:A:298:THR:HG22	1:A:299:MET:HE2	1.95	0.48
1:B:477:ASN:ND2	1:B:482:GLY:H	1.98	0.48
1:A:123:ILE:HD12	1:A:123:ILE:N	2.28	0.48
1:B:603:TYR:CE1	1:B:607:MET:HE3	2.49	0.48
1:B:643:PHE:CE1	1:B:656:ILE:HD11	2.48	0.48
1:B:357:ILE:HG22	1:B:407:MET:CE	2.44	0.48
1:B:452:LYS:HD3	1:B:474:ILE:CD1	2.44	0.48
1:A:521:SER:OG	1:A:523:HIS:HD2	1.97	0.48
1:A:712:LEU:HD23	1:A:712:LEU:C	2.39	0.48
1:B:667:ASP:O	1:B:671:VAL:HG23	2.14	0.48
1:A:7:ASP:O	1:A:23:GLU:HA	2.14	0.48
1:B:86:ILE:HD13	1:B:86:ILE:C	2.38	0.47
1:A:700:GLU:HG2	4:A:2385:HOH:O	2.13	0.47
1:A:450:ASN:HB3	4:A:2337:HOH:O	2.14	0.47
1:B:218:LYS:NZ	1:B:220:HIS:HD2	2.12	0.47
1:B:633:THR:HG21	1:B:635:ASP:HB2	1.96	0.47
1:B:740:ASP:O	1:B:744:ILE:HG12	2.14	0.47
1:B:20:ASN:ND2	4:B:2246:HOH:O	2.47	0.47
1:B:173:GLU:HG2	1:B:190:ILE:HD12	1.96	0.47
1:A:341:GLU:CD	1:A:341:GLU:H	2.21	0.47
1:A:370:PHE:O	1:A:374:ILE:HG12	2.15	0.47
1:B:32:ILE:CD1	1:B:64:GLY:HA3	2.45	0.47
1:B:357:ILE:HG22	1:B:407:MET:HE1	1.96	0.47
1:B:432:GLN:HE22	1:B:445:TRP:N	2.07	0.47
1:B:753:ILE:C	1:B:753:ILE:HD12	2.40	0.47
1:A:14:ILE:H	1:A:14:ILE:CD1	2.19	0.47
1:B:241:ARG:HG3	4:B:2193:HOH:O	2.15	0.47
1:A:421:LEU:HD23	1:A:430:MET:HB3	1.97	0.47
1:B:332:ILE:HD11	1:B:353:LYS:CD	2.25	0.47
1:A:290:PHE:CE1	1:A:374:ILE:HD12	2.49	0.46
1:A:663:LYS:HD2	1:A:697:PRO:HG3	1.97	0.46
1:B:402:PRO:O	1:B:406:VAL:HG23	2.15	0.46
1:A:473:LEU:HD23	1:A:473:LEU:C	2.41	0.46
1:B:134:ILE:HD12	1:B:134:ILE:N	2.25	0.46
1:B:253:VAL:CG2	1:B:583:GLU:HG2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ILE:N	1:B:332:ILE:CD1	2.78	0.46
1:B:574:MET:CE	1:B:589:LEU:HD12	2.45	0.46
1:B:32:ILE:HD13	1:B:63:PRO:O	2.15	0.46
1:B:452:LYS:HD3	1:B:474:ILE:HD12	1.96	0.46
1:B:509:ILE:HD13	1:B:544:VAL:HA	1.97	0.46
1:B:731:ILE:N	1:B:732:PRO:HD2	2.31	0.46
1:B:3:VAL:HG11	1:B:6:TYR:CE2	2.51	0.46
1:B:475:LYS:NZ	1:B:507:ASP:HB3	2.30	0.46
1:B:573:ARG:NE	1:B:573:ARG:HA	2.30	0.46
1:B:642:LYS:HA	1:B:645:SER:HB3	1.98	0.46
1:B:33:VAL:O	1:B:33:VAL:HG13	2.16	0.46
1:A:146:GLU:HG2	4:A:2113:HOH:O	2.16	0.45
1:B:142:ILE:HD12	1:B:150:VAL:CG2	2.26	0.45
1:B:328:ASN:HB3	1:B:755:MET:HE1	1.98	0.45
1:B:422:LYS:HG3	1:B:422:LYS:O	2.16	0.45
1:A:86:ILE:HD11	1:A:96:ILE:CG2	2.46	0.45
1:A:751:LYS:HA	1:A:754:SER:OG	2.17	0.45
1:B:421:LEU:HD11	1:B:476:ILE:HD12	1.97	0.45
1:B:685:MET:HE3	1:B:713:VAL:HG22	1.97	0.45
1:B:698:GLY:O	1:B:702:ILE:HG12	2.17	0.45
1:A:505:PRO:HD3	2:A:1007:SO4:O1	2.17	0.45
1:B:282:ASN:HD22	1:B:282:ASN:H	1.64	0.45
1:A:509:ILE:O	1:A:509:ILE:HD13	2.17	0.45
1:B:41:ILE:N	1:B:41:ILE:HD12	2.31	0.45
1:B:248:ALA:HB3	1:B:251:SER:OG	2.17	0.45
1:B:247:ILE:N	1:B:247:ILE:HD12	2.32	0.45
1:B:276:VAL:HG21	1:B:378:LEU:HA	1.99	0.45
1:B:474:ILE:HD11	1:B:503:LEU:HD23	1.99	0.45
1:B:540:GLU:HB3	1:B:576:PHE:CE2	2.52	0.45
1:B:194:TYR:N	1:B:195:PRO:HD2	2.31	0.45
1:B:278:MET:HE2	4:B:2028:HOH:O	2.16	0.45
1:B:493:PHE:CE2	1:B:532:ARG:HB3	2.51	0.45
1:A:416:TYR:HE2	1:A:485:ARG:HG3	1.82	0.45
1:B:299:MET:CE	1:B:302:LEU:HD12	2.47	0.45
1:B:682:LYS:HE3	1:B:717:PHE:CE1	2.52	0.45
1:A:724:SER:O	1:A:727:VAL:HG22	2.16	0.45
1:B:167:ILE:HD12	1:B:167:ILE:N	2.32	0.45
1:A:32:ILE:O	1:A:61:ARG:HA	2.17	0.44
1:A:708:ARG:HG3	4:A:2122:HOH:O	2.18	0.44
1:A:86:ILE:C	1:A:86:ILE:HD13	2.42	0.44
1:A:709:ILE:O	1:A:713:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:HIS:NE2	1:B:349:ILE:HD12	2.32	0.44
1:A:184:LEU:HB2	1:A:196:LEU:HD21	1.99	0.44
1:A:357:ILE:CD1	1:A:357:ILE:C	2.90	0.44
1:B:35:ASP:O	1:B:110:PRO:HA	2.18	0.44
1:A:505:PRO:HG2	4:A:2060:HOH:O	2.17	0.44
1:B:359:ARG:HH22	1:B:481:ALA:HA	1.80	0.44
1:A:54:THR:O	1:A:60:VAL:HA	2.16	0.44
1:B:7:ASP:O	1:B:23:GLU:HA	2.17	0.44
1:B:140:LYS:HB2	1:B:153:GLN:HG3	1.99	0.44
1:B:86:ILE:O	1:B:86:ILE:HG23	2.17	0.44
1:B:134:ILE:CD1	1:B:134:ILE:N	2.80	0.44
1:B:361:ILE:HD11	1:B:403:VAL:HG13	2.00	0.44
1:A:556:ARG:HD2	1:A:599:VAL:CG1	2.48	0.44
1:A:574:MET:HE1	1:A:593:SER:HB2	1.99	0.44
1:A:345:ILE:C	1:A:347:ASP:H	2.26	0.44
1:A:705:ASN:HB3	1:A:709:ILE:CD1	2.48	0.44
1:B:164:TYR:CE2	1:B:222:ILE:HD13	2.53	0.44
1:A:114:HIS:CD2	1:A:116:ALA:HB3	2.53	0.44
1:B:44:MET:HG2	1:B:45:LYS:N	2.32	0.44
1:B:505:PRO:O	1:B:509:ILE:HG12	2.18	0.44
1:A:83:LEU:HG	1:A:87:TYR:CZ	2.53	0.43
1:A:190:ILE:N	1:A:190:ILE:HD12	2.32	0.43
1:B:427:LYS:HG2	1:B:467:SER:OG	2.18	0.43
1:B:428:ILE:HG13	1:B:470:ALA:HB2	1.99	0.43
1:A:129:LYS:HG2	1:A:144:VAL:HG13	2.00	0.43
1:A:570:CYS:SG	1:A:595:LEU:HD13	2.58	0.43
1:A:681:LYS:HB3	1:A:683:GLN:HG2	2.01	0.43
1:A:720:ASN:HA	4:A:2106:HOH:O	2.17	0.43
1:B:153:GLN:HG2	4:B:2294:HOH:O	2.18	0.43
1:B:284:LEU:O	1:B:284:LEU:HD22	2.18	0.43
1:B:545:ILE:HD12	1:B:573:ARG:CD	2.48	0.43
1:B:727:VAL:O	1:B:731:ILE:HG12	2.18	0.43
1:A:85:GLY:O	1:A:98:THR:HA	2.18	0.43
1:A:20:ASN:ND2	4:A:2434:HOH:O	2.52	0.43
1:A:696:LEU:N	1:A:697:PRO:HD2	2.34	0.43
1:A:136:ASN:ND2	1:A:164:TYR:H	2.17	0.43
1:B:85:GLY:O	1:B:98:THR:HA	2.19	0.43
1:B:421:LEU:HD21	1:B:476:ILE:CD1	2.49	0.43
1:B:775:ARG:HG2	1:B:775:ARG:HH21	1.83	0.43
1:A:675:VAL:HG22	1:A:680:ILE:HB	2.00	0.43
1:B:275:LEU:HD22	1:B:383:PHE:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LEU:O	1:A:84:SER:HB2	2.17	0.43
1:A:778:ALA:HB2	4:A:2285:HOH:O	2.17	0.43
1:B:99:HIS:NE2	1:B:101:GLU:HB3	2.34	0.43
1:A:137:MET:HG2	1:A:155:THR:HG22	2.01	0.42
1:B:281:TRP:O	1:B:284:LEU:HB2	2.19	0.42
1:A:173:GLU:HG3	1:A:190:ILE:HG21	2.00	0.42
1:A:392:TRP:CH2	1:A:407:MET:HE2	2.54	0.42
1:B:656:ILE:O	1:B:659:PHE:HB2	2.19	0.42
1:B:769:LYS:O	1:B:773:ARG:HG3	2.19	0.42
1:B:725:ARG:HG3	1:B:725:ARG:HH21	1.84	0.42
1:A:527:GLU:CG	1:A:531:GLN:HE22	2.33	0.42
1:A:369:GLU:OE1	1:A:399:SER:HA	2.19	0.42
1:B:100:PHE:CD2	1:B:105:ALA:HA	2.55	0.42
1:B:425:GLY:C	1:B:427:LYS:N	2.78	0.42
1:B:527:GLU:OE2	1:B:530:ARG:NH1	2.53	0.42
1:A:286:LEU:HD22	1:A:286:LEU:O	2.20	0.42
1:A:453:LYS:HB2	1:A:456:GLY:O	2.20	0.42
1:A:719:GLY:O	1:A:752:ASN:HB3	2.19	0.42
1:B:86:ILE:CG1	1:B:108:MET:HE3	2.50	0.42
1:A:101:GLU:O	1:A:102:ALA:HB3	2.20	0.42
1:A:18:THR:HA	1:A:78:LYS:HA	2.02	0.42
1:A:86:ILE:HG23	1:A:86:ILE:O	2.19	0.42
1:A:332:ILE:HD12	1:A:411:ILE:HA	2.01	0.42
1:B:425:GLY:C	1:B:427:LYS:H	2.27	0.42
1:B:648:ARG:HG2	1:B:650:GLU:H	1.84	0.42
1:A:177:TYR:OH	1:A:204:GLU:HG3	2.20	0.41
1:A:276:VAL:HG21	1:A:378:LEU:HA	2.02	0.41
1:A:452:LYS:HE3	1:A:478:ALA:CB	2.45	0.41
1:B:97:THR:CG2	1:B:164:TYR:OH	2.68	0.41
1:A:59:THR:HG22	1:A:60:VAL:N	2.35	0.41
1:B:280:TRP:HB3	1:B:282:ASN:ND2	2.35	0.41
1:B:559:THR:OG1	1:B:560:HIS:N	2.54	0.41
1:B:575:GLN:C	1:B:575:GLN:CD	2.88	0.41
1:B:774:ILE:C	1:B:776:GLN:H	2.27	0.41
1:B:79:VAL:HG22	1:B:86:ILE:HD12	2.03	0.41
1:B:643:PHE:CZ	1:B:656:ILE:HD11	2.54	0.41
1:B:779:VAL:C	1:B:780:LYS:HG3	2.45	0.41
1:A:313:PHE:CD2	1:A:509:ILE:HD12	2.56	0.41
1:B:97:THR:HG22	1:B:164:TYR:CE1	2.55	0.41
1:B:509:ILE:HD11	1:B:544:VAL:N	2.35	0.41
1:B:558:LEU:HG	1:B:736:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ILE:HD12	1:A:131:TYR:CB	2.51	0.41
1:B:69:GLN:HG3	1:B:71:ILE:CD1	2.45	0.41
1:B:165:VAL:HG12	1:B:167:ILE:CD1	2.50	0.41
1:B:681:LYS:HB2	1:B:684:ASP:CG	2.45	0.41
1:A:395:ILE:N	1:A:395:ILE:HD12	2.36	0.41
1:B:528:THR:O	1:B:532:ARG:CG	2.68	0.41
1:A:240:PHE:CG	1:A:245:MET:HE3	2.56	0.41
1:A:530:ARG:O	1:A:534:ARG:HG3	2.21	0.41
1:B:476:ILE:HG22	1:B:477:ASN:N	2.35	0.41
1:A:218:LYS:HZ3	1:A:220:HIS:HD2	1.68	0.41
1:A:219:MET:HE2	1:A:270:GLN:HG3	2.03	0.41
1:A:327:LYS:HD3	4:A:2058:HOH:O	2.20	0.41
1:A:342:ILE:HD13	1:A:342:ILE:C	2.46	0.41
1:A:424:ASN:OD1	1:A:427:LYS:HB3	2.20	0.41
1:A:649:ASP:OD1	1:A:652:ARG:NH2	2.54	0.41
1:B:67:GLN:O	1:B:68:PRO:C	2.64	0.41
1:B:134:ILE:HD13	1:B:170:PHE:HE2	1.77	0.41
1:B:184:LEU:HD22	1:B:190:ILE:HD11	2.01	0.41
1:B:349:ILE:O	1:B:353:LYS:HB3	2.20	0.41
1:B:422:LYS:CD	1:B:429:THR:HG23	2.51	0.41
1:B:428:ILE:O	1:B:468:ILE:HD13	2.21	0.41
1:A:233:GLU:HA	1:A:238:ILE:CD1	2.27	0.41
1:B:196:LEU:HD23	1:B:196:LEU:HA	1.91	0.41
1:B:332:ILE:HD12	1:B:349:ILE:CG2	2.51	0.41
1:A:697:PRO:O	1:A:700:GLU:HB2	2.21	0.40
1:B:137:MET:HB3	1:B:138:PRO:CD	2.51	0.40
1:B:332:ILE:N	1:B:332:ILE:HD12	2.36	0.40
1:A:361:ILE:HG13	1:A:407:MET:CG	2.51	0.40
1:A:577:LEU:HD13	1:A:589:LEU:HA	2.03	0.40
1:A:583:GLU:HB3	4:A:2252:HOH:O	2.21	0.40
1:B:492:THR:HA	1:B:495:ASP:OD1	2.21	0.40
1:B:11:ASP:OD1	1:B:147:ARG:NH1	2.54	0.40
1:B:685:MET:HE1	1:B:717:PHE:HE2	1.85	0.40
1:A:11:ASP:OD1	1:A:11:ASP:C	2.65	0.40
1:A:43:TRP:CZ3	1:A:45:LYS:HE3	2.56	0.40
1:A:262:VAL:O	1:A:265:HIS:HB3	2.21	0.40
1:B:86:ILE:HD11	1:B:96:ILE:CG2	2.51	0.40
1:B:127:ILE:HD13	1:B:127:ILE:H	1.86	0.40
1:B:556:ARG:NH1	1:B:598:MET:HE3	2.37	0.40
1:B:656:ILE:HD12	1:B:680:ILE:HG13	2.04	0.40
1:B:685:MET:HE1	1:B:713:VAL:HG22	2.02	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	778/780 (100%)	729 (94%)	41 (5%)	8 (1%)	12	15
1	B	778/780 (100%)	716 (92%)	45 (6%)	17 (2%)	5	4
All	All	1556/1560 (100%)	1445 (93%)	86 (6%)	25 (2%)	7	7

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	ALA
1	B	102	ALA
1	B	341	GLU
1	B	342	ILE
1	B	347	ASP
1	B	423	ARG
1	B	83	LEU
1	B	346	PHE
1	B	422	LYS
1	B	475	LYS
1	A	91	ARG
1	A	778	ALA
1	B	101	GLU
1	B	464	ASP
1	B	718	THR
1	A	84	SER
1	A	101	GLU
1	A	339	PRO
1	A	718	THR
1	B	678	THR
1	B	721	ARG
1	B	720	ASN

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Mol	Chain	Res	Type
1	A	648	ARG
1	B	424	ASN
1	B	339	PRO

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	677/677 (100%)	641 (95%)	36 (5%)	20	30
1	B	677/677 (100%)	636 (94%)	41 (6%)	17	24
All	All	1354/1354 (100%)	1277 (94%)	77 (6%)	18	27

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	33	VAL
1	A	86	ILE
1	A	129	LYS
1	A	151	GLU
1	A	187	LEU
1	A	198	MET
1	A	232	MET
1	A	247	ILE
1	A	275	LEU
1	A	282	ASN
1	A	284	LEU
1	A	286	LEU
1	A	341	GLU
1	A	342	ILE
1	A	361	ILE
1	A	395	ILE
1	A	417	PRO
1	A	447	VAL
1	A	462	LEU

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Mol	Chain	Res	Type
1	A	487	LEU
1	A	509	ILE
1	A	519	LEU
1	A	531	GLN
1	A	555	LEU
1	A	595	LEU
1	A	596	TYR
1	A	607	MET
1	A	636	LEU
1	A	647	ASP
1	A	686	ILE
1	A	696	LEU
1	A	709	ILE
1	A	720	ASN
1	A	764	LEU
1	A	770	LEU
1	B	1	MET
1	B	58	GLN
1	B	86	ILE
1	B	92	GLU
1	B	97	THR
1	B	106	ARG
1	B	127	ILE
1	B	134	ILE
1	B	250	ASN
1	B	266	GLU
1	B	275	LEU
1	B	282	ASN
1	B	284	LEU
1	B	286	LEU
1	B	288	GLU
1	B	332	ILE
1	B	361	ILE
1	B	379	ASN
1	B	422	LYS
1	B	424	ASN
1	B	429	THR
1	B	430	MET
1	B	468	ILE
1	B	471	ASP
1	B	474	ILE
1	B	485	ARG

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Mol	Chain	Res	Type
1	B	487	LEU
1	B	519	LEU
1	B	530	ARG
1	B	532	ARG
1	B	555	LEU
1	B	559	THR
1	B	581	GLN
1	B	583	GLU
1	B	594	ARG
1	B	595	LEU
1	B	642	LYS
1	B	650	GLU
1	B	679	GLU
1	B	764	LEU
1	B	777	THR

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	20	ASN
1	A	40	GLN
1	A	42	ASN
1	A	58	GLN
1	A	69	GLN
1	A	114	HIS
1	A	136	ASN
1	A	153	GLN
1	A	220	HIS
1	A	234	ASN
1	A	258	ASN
1	A	261	ASN
1	A	344	GLN
1	A	379	ASN
1	A	432	GLN
1	A	477	ASN
1	A	499	HIS
1	A	523	HIS
1	A	531	GLN
1	A	542	HIS
1	A	551	GLN
1	A	581	GLN
1	A	720	ASN

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Mol	Chain	Res	Type
1	A	776	GLN
1	B	20	ASN
1	B	40	GLN
1	B	42	ASN
1	B	58	GLN
1	B	114	HIS
1	B	136	ASN
1	B	220	HIS
1	B	234	ASN
1	B	258	ASN
1	B	282	ASN
1	B	328	ASN
1	B	385	ASN
1	B	432	GLN
1	B	438	ASN
1	B	450	ASN
1	B	477	ASN
1	B	535	ASN
1	B	551	GLN
1	B	705	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 2 are monoatomic - leaving 17 for Mogul analysis.

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	A	1001	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	B	1004	-	4,4,4	0.43	0	6,6,6	0.09	0
2	SO4	A	1015	-	4,4,4	0.41	0	6,6,6	0.10	0
2	SO4	A	1009	-	4,4,4	0.40	0	6,6,6	0.07	0
2	SO4	A	1003	-	4,4,4	0.38	0	6,6,6	0.09	0
2	SO4	B	1013	-	4,4,4	0.38	0	6,6,6	0.08	0
2	SO4	A	1007	-	4,4,4	0.38	0	6,6,6	0.06	0
2	SO4	A	1010	-	4,4,4	0.42	0	6,6,6	0.08	0
2	SO4	B	1011	-	4,4,4	0.43	0	6,6,6	0.07	0
2	SO4	A	1006	-	4,4,4	0.36	0	6,6,6	0.09	0
2	SO4	A	1016	-	4,4,4	0.44	0	6,6,6	0.09	0
2	SO4	A	1008	-	4,4,4	0.37	0	6,6,6	0.08	0
2	SO4	A	1014	-	4,4,4	0.40	0	6,6,6	0.09	0
2	SO4	A	1017	-	4,4,4	0.41	0	6,6,6	0.08	0
2	SO4	B	1012	-	4,4,4	0.42	0	6,6,6	0.09	0
2	SO4	A	1005	-	4,4,4	0.37	0	6,6,6	0.09	0
2	SO4	A	1002	-	4,4,4	0.43	0	6,6,6	0.08	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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1007	SO4	1	0
2	A	1017	SO4	1	0
2	A	1005	SO4	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	780/780 (100%)	0.13	26 (3%)	49	51	18, 34, 58, 67	1 (0%)
1	B	780/780 (100%)	0.25	37 (4%)	36	38	19, 38, 60, 68	4 (0%)
All	All	1560/1560 (100%)	0.19	63 (4%)	42	44	18, 36, 59, 68	5 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	779	VAL	8.5
1	A	346	PHE	5.7
1	B	720	ASN	5.5
1	B	778	ALA	5.4
1	B	345	ILE	5.2
1	B	779	VAL	5.2
1	B	248	ALA	4.7
1	A	718	THR	4.3
1	B	424	ASN	4.1
1	B	425	GLY	4.0
1	A	65	ASP	3.9
1	A	345	ILE	3.9
1	A	778	ALA	3.8
1	A	57	GLY	3.8
1	B	306	TRP	3.3
1	A	248	ALA	3.3
1	B	474	ILE	3.2
1	B	93	ASN	3.1
1	B	777	THR	3.1
1	A	720	ASN	3.1
1	B	718	THR	2.9
1	A	66	SER	2.8
1	A	247	ILE	2.8
1	A	349	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	780	LYS	2.7
1	B	614	PHE	2.7
1	B	247	ILE	2.7
1	B	780	LYS	2.7
1	A	249	GLU	2.7
1	A	191	ARG	2.7
1	B	471	ASP	2.6
1	B	347	ASP	2.6
1	B	426	ARG	2.6
1	A	338	ASP	2.6
1	B	346	PHE	2.6
1	A	252	ALA	2.5
1	B	649	ASP	2.5
1	B	454	LYS	2.5
1	A	777	THR	2.5
1	B	349	ILE	2.5
1	B	428	ILE	2.5
1	B	343	SER	2.4
1	A	342	ILE	2.4
1	B	344	GLN	2.4
1	B	427	LYS	2.3
1	A	719	GLY	2.3
1	B	332	ILE	2.3
1	B	509	ILE	2.3
1	B	675	VAL	2.2
1	B	250	ASN	2.2
1	B	721	ARG	2.2
1	B	470	ALA	2.2
1	A	337	ARG	2.2
1	A	253	VAL	2.2
1	A	339	PRO	2.2
1	A	64	GLY	2.1
1	A	343	SER	2.1
1	A	424	ASN	2.1
1	B	341	GLU	2.1
1	B	190	ILE	2.1
1	B	340	ASP	2.0
1	B	646	VAL	2.0
1	B	455	ASP	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($\text{\AA}^2$)	Q<0.9
2	SO4	A	1017	5/5	0.64	0.23	89,89,90,91	0
2	SO4	A	1016	5/5	0.71	0.17	73,74,76,77	0
2	SO4	B	1012	5/5	0.72	0.22	85,85,87,87	0
2	SO4	A	1014	5/5	0.79	0.22	78,79,79,80	0
2	SO4	B	1011	5/5	0.79	0.31	78,78,79,82	0
2	SO4	A	1008	5/5	0.79	0.19	78,80,80,80	0
2	SO4	A	1015	5/5	0.80	0.17	73,73,74,74	0
2	SO4	B	1004	5/5	0.81	0.20	76,78,78,79	0
2	SO4	A	1007	5/5	0.81	0.22	82,82,83,83	0
2	SO4	A	1002	5/5	0.81	0.15	80,81,81,83	0
2	SO4	A	1003	5/5	0.82	0.18	74,75,75,77	0
2	SO4	A	1010	5/5	0.85	0.27	71,72,74,74	0
2	SO4	A	1009	5/5	0.87	0.16	76,76,78,78	0
2	SO4	B	1013	5/5	0.89	0.12	76,76,77,77	0
2	SO4	A	1001	5/5	0.90	0.11	58,59,60,60	0
2	SO4	A	1005	5/5	0.92	0.09	66,66,68,68	0
2	SO4	A	1006	5/5	0.94	0.11	61,62,63,63	0
3	ZN	B	2002	1/1	0.98	0.06	30,30,30,30	0
3	ZN	A	2001	1/1	1.00	0.08	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.