Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:02 PM GMT

PDB ID	:	1W8Y
Title	:	CRYSTAL STRUCTURE OF THE NITROCEFIN ACYL-DD-PEPTIDASE FROM ACTINOMADURA R39.
Authors	:	Sauvage, E.; Herman, R.; Petrella, S.; Duez, C.; Frere, J.M.; Charlier, P.
Deposited on	:	2004-10-01
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

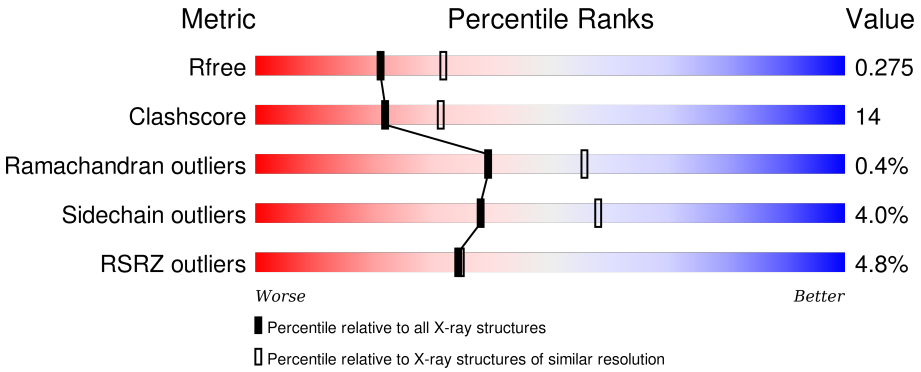
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	489	8% 64% 29%
1	B	489	3% 68% 26% 5%
1	C	489	4% 65% 29% 5%
1	D	489	4% 73% 21%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	D	510	-	-	-	X
3	MG	D	511	-	-	-	X

2 Entry composition

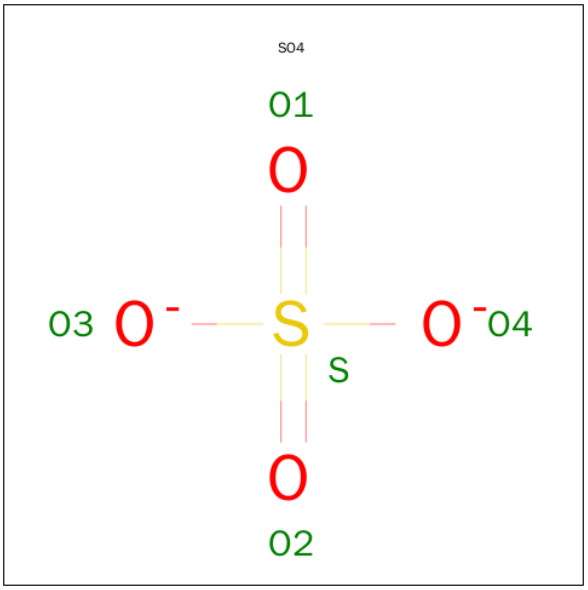
There are 5 unique types of molecules in this entry. The entry contains 14391 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-ALANYL-D-ALANINE CARBOXYPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	1
			3353	2076	565	706	6			
1	B	466	Total	C	N	O	S	0	0	1
			3344	2071	564	703	6			
1	C	466	Total	C	N	O	S	0	0	1
			3344	2071	564	703	6			
1	D	467	Total	C	N	O	S	0	0	1
			3353	2076	565	706	6			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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		

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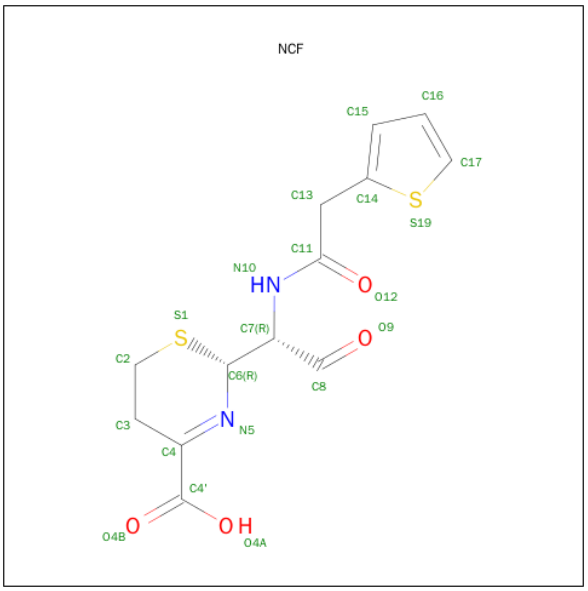
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total Mg 2 2	0	0
3	D	2	Total Mg 2 2	0	0

- Molecule 4 is (2R)-2-{(1R)-2-OXO-1-[(2-THIENYLACETYL)AMINO]ETHYL}-5,6-DIHYDRO-2H-1,3-THIAZINE-4-CARBOXYLIC ACID (three-letter code: NCF) (formula: $C_{13}H_{14}N_2O_4S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			21	13	2	4	2		
4	B	1	Total	C	N	O	S	0	0
			21	13	2	4	2		
4	C	1	Total	C	N	O	S	0	0
			21	13	2	4	2		
4	D	1	Total	C	N	O	S	0	0
			21	13	2	4	2		

- Molecule 5 is water.

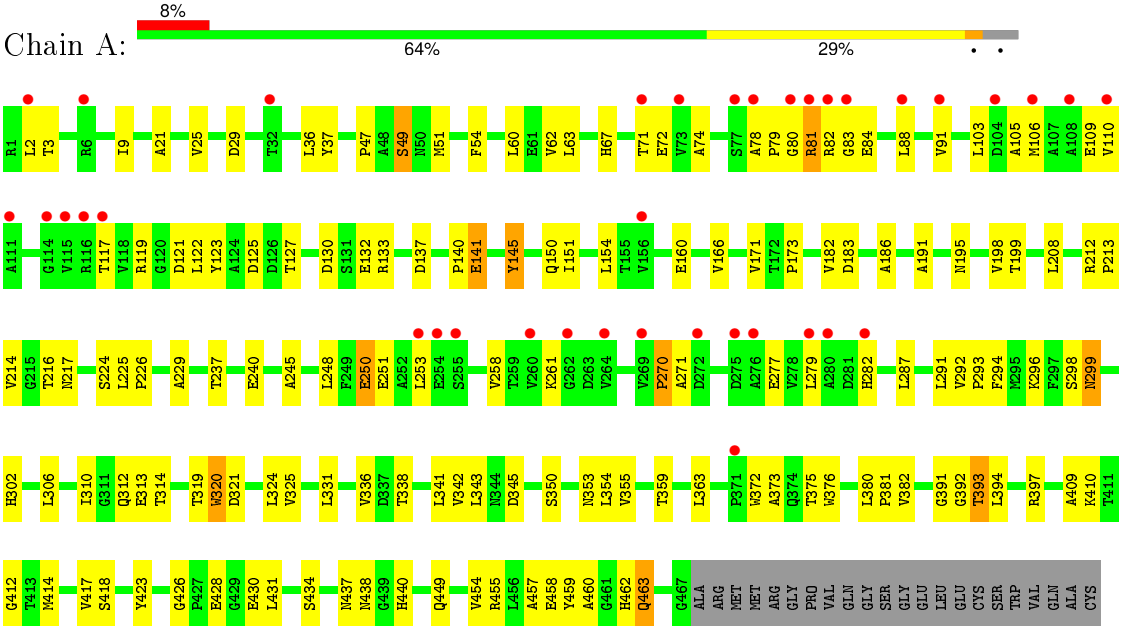
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	191	Total	O	0	0
			191	191		
5	B	222	Total	O	0	0
			222	222		
5	C	198	Total	O	0	0
			198	198		
5	D	218	Total	O	0	0
			218	218		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

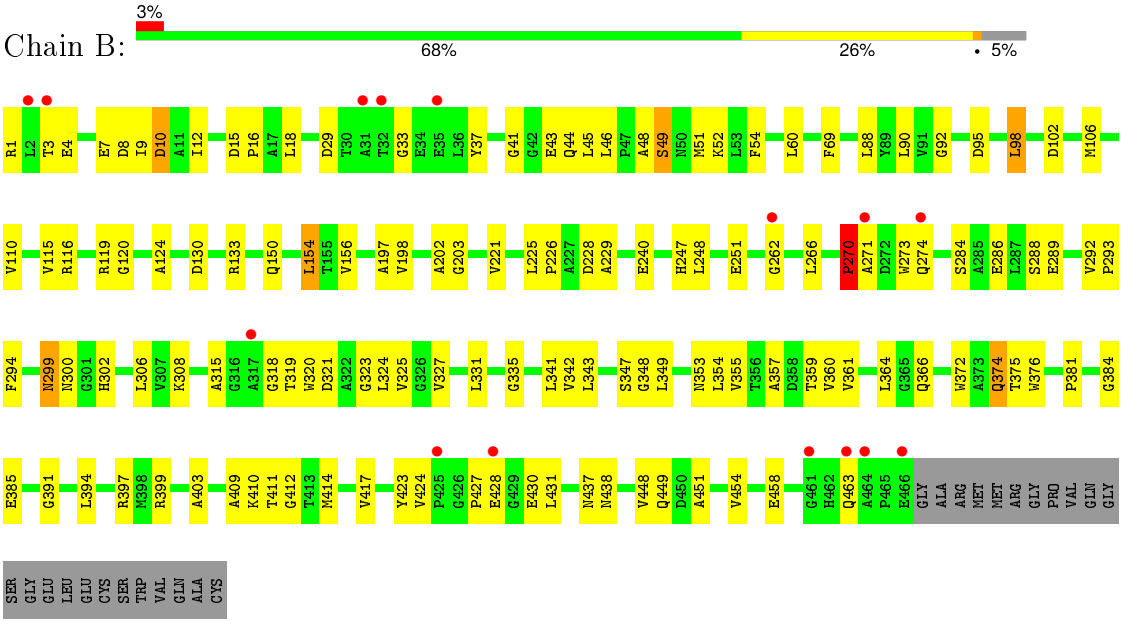
- Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE

Chain A:



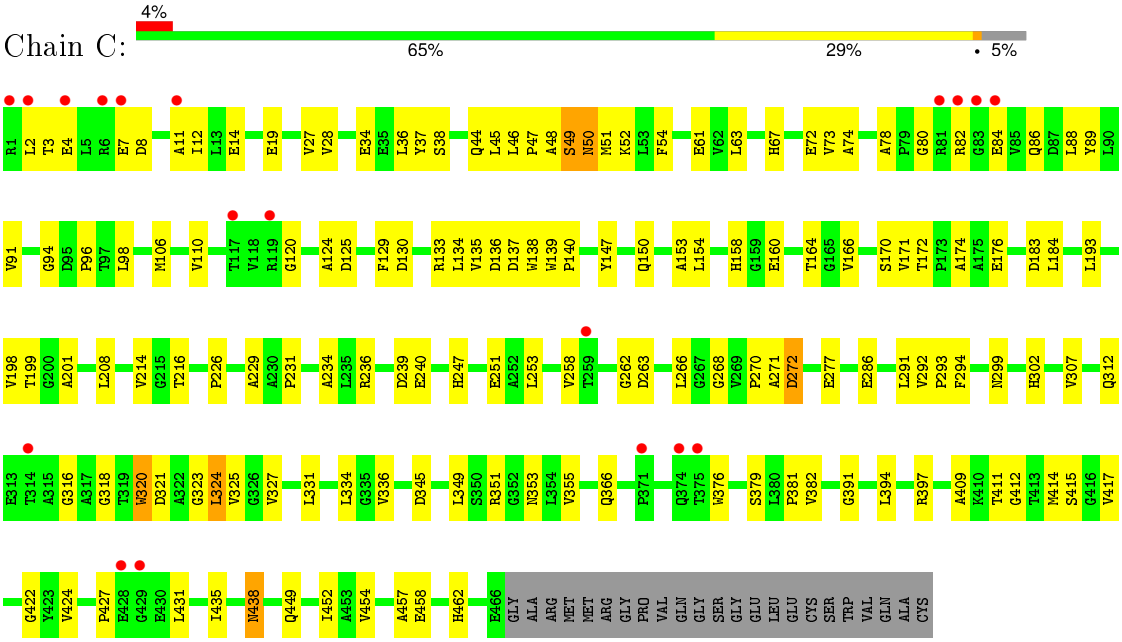
- Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE

Chain B:



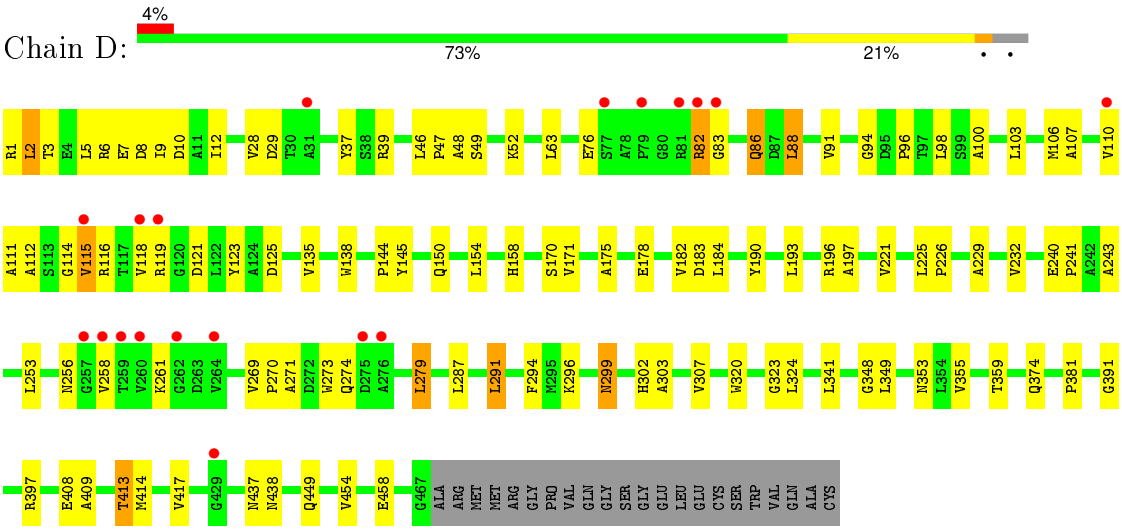
• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE

Chain C:



• Molecule 1: D-ALANYL-D-ALANINE CARBOXYPEPTIDASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	103.49Å 94.36Å 107.20Å 90.00° 94.58° 90.00°	Depositor
Resolution (Å)	19.94 – 2.40 40.66 – 2.40	Depositor EDS
% Data completeness (in resolution range)	86.3 (19.94-2.40) 86.5 (40.66-2.40)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.277 0.217 , 0.275	Depositor DCC
R_{free} test set	3534 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	35.0	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 54.8	EDS
Estimated twinning fraction	0.028 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	2 of 69686 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	14391	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.73% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, SO4, NCF

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	0.42	1/3412 (0.0%)	0.63	0/4668
1	B	0.42	1/3403 (0.0%)	0.63	0/4656
1	C	0.40	1/3403 (0.0%)	0.63	0/4656
1	D	0.44	1/3412 (0.0%)	0.65	0/4668
All	All	0.42	4/13630 (0.0%)	0.64	0/18648

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	49	SER	CB-OG	-12.35	1.26	1.42
1	D	49	SER	CB-OG	-11.99	1.26	1.42
1	C	49	SER	CB-OG	-11.92	1.26	1.42
1	A	49	SER	CB-OG	-11.86	1.26	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	145	TYR	Sidechain

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	3353	0	3200	114	0
1	B	3344	0	3194	87	0
1	C	3344	0	3194	91	0
1	D	3353	0	3200	76	0
2	A	20	0	0	2	0
2	B	20	0	0	0	0
2	C	20	0	0	1	0
2	D	20	0	0	0	0
3	A	2	0	0	0	0
3	D	2	0	0	0	0
4	A	21	0	12	1	0
4	B	21	0	12	0	0
4	C	21	0	12	1	0
4	D	21	0	12	1	0
5	A	191	0	0	7	0
5	B	222	0	0	8	0
5	C	198	0	0	6	0
5	D	218	0	0	5	0
All	All	14391	0	12836	366	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 14.

All (366) 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:226:PRO:HG2	1:A:229:ALA:HB2	1.26	1.16
1:B:226:PRO:HB3	5:B:2126:HOH:O	1.60	1.00
1:C:226:PRO:HG2	1:C:229:ALA:HB2	1.47	0.95
1:D:150:GLN:HE22	1:D:240:GLU:H	1.25	0.84
1:A:80:GLY:HA3	1:B:315:ALA:HA	1.59	0.84
1:B:1:ARG:HB3	1:B:4:GLU:HG3	1.62	0.82
1:A:2:LEU:HG	1:A:459:TYR:OH	1.81	0.81
1:B:124:ALA:HB3	1:B:266:LEU:HD23	1.65	0.78
1:D:144:PRO:HG2	1:D:145:TYR:CE1	2.19	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:ASN:HD22	1:A:302:HIS:H	1.31	0.77
1:D:150:GLN:NE2	1:D:240:GLU:H	1.85	0.74
1:B:454:VAL:O	1:B:458:GLU:HG3	1.89	0.73
1:C:394:LEU:HD11	1:C:411:THR:HG23	1.70	0.72
1:B:12:ILE:HG22	1:B:448:VAL:HG13	1.72	0.71
1:C:2:LEU:HD23	1:C:2:LEU:O	1.91	0.70
1:B:15:ASP:OD1	1:B:16:PRO:HD2	1.92	0.70
1:B:343:LEU:N	1:B:343:LEU:HD12	2.07	0.70
1:B:288:SER:HB2	1:B:375:THR:HG21	1.72	0.70
1:A:2:LEU:HD21	1:A:36:LEU:HD22	1.74	0.69
1:A:106:MET:O	1:A:110:VAL:HG23	1.93	0.69
1:A:397:ARG:HH12	1:A:449:GLN:HE21	1.40	0.69
1:A:414:MET:HB3	1:A:417:VAL:HB	1.75	0.69
1:B:397:ARG:HH12	1:B:449:GLN:HE21	1.41	0.68
1:C:253:LEU:HB3	1:C:258:VAL:HB	1.75	0.67
1:A:150:GLN:NE2	1:A:240:GLU:H	1.93	0.67
1:C:381:PRO:HB2	1:C:394:LEU:HD13	1.77	0.66
1:A:341:LEU:HG	1:A:359:THR:HG21	1.76	0.66
1:C:51:MET:HE2	1:C:353:ASN:HB3	1.78	0.66
1:B:414:MET:HG2	1:B:417:VAL:HB	1.78	0.66
1:A:125:ASP:OD2	1:A:127:THR:HG23	1.96	0.65
1:A:454:VAL:O	1:A:458:GLU:HG3	1.95	0.65
1:B:119:ARG:HG2	1:B:119:ARG:HH11	1.61	0.65
1:B:90:LEU:HG	1:B:154:LEU:HD11	1.78	0.65
1:D:83:GLY:HA3	1:D:116:ARG:HB3	1.79	0.65
1:C:129:PHE:HB2	1:C:153:ALA:HB2	1.79	0.65
1:A:426:GLY:HA3	1:A:460:ALA:HB1	1.78	0.65
1:C:49:SER:HB2	1:C:412:GLY:HA2	1.78	0.64
1:A:62:VAL:HG11	1:A:310:ILE:HG23	1.79	0.64
1:B:92:GLY:HA3	1:B:154:LEU:HG	1.81	0.63
1:A:298:SER:HG	1:A:410:LYS:HZ1	1.43	0.63
1:C:351:ARG:HH12	1:C:415:SER:HB2	1.63	0.63
1:A:82:ARG:HB2	1:A:84:GLU:HG3	1.81	0.62
1:D:115:VAL:HG12	1:D:258:VAL:HG13	1.81	0.62
1:A:341:LEU:CD2	1:A:355:VAL:HG12	2.30	0.62
1:A:49:SER:HB2	1:A:412:GLY:HA2	1.82	0.61
1:A:51:MET:HE2	1:A:353:ASN:HB3	1.81	0.61
1:B:397:ARG:HH12	1:B:449:GLN:NE2	1.97	0.61
1:C:8:ASP:O	1:C:12:ILE:HG13	1.99	0.61
1:D:52:LYS:HD3	1:D:294:PHE:CE2	2.36	0.61
1:B:156:VAL:HG21	1:B:248:LEU:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:PRO:C	1:C:272:ASP:H	2.05	0.60
1:A:119:ARG:CZ	1:A:261:LYS:HE3	2.32	0.60
1:A:282:HIS:HA	2:A:501:SO4:O1	2.00	0.60
1:C:124:ALA:HB3	1:C:266:LEU:HD23	1.82	0.60
1:C:106:MET:O	1:C:110:VAL:HG23	2.01	0.60
1:D:86:GLN:O	1:D:118:VAL:HG13	2.03	0.59
1:C:45:LEU:HD22	1:C:438:ASN:HB2	1.85	0.59
1:B:197:ALA:HB2	1:B:221:VAL:HG12	1.84	0.59
1:C:414:MET:HB2	1:C:417:VAL:HB	1.84	0.59
1:C:46:LEU:HD13	1:C:353:ASN:O	2.03	0.58
1:C:351:ARG:NH1	1:C:415:SER:HB2	2.18	0.58
1:A:198:VAL:CG1	1:A:224:SER:HB3	2.33	0.58
1:C:198:VAL:HG22	1:C:199:THR:N	2.19	0.58
1:A:198:VAL:HG22	1:A:199:THR:N	2.19	0.58
1:A:154:LEU:CD1	1:A:245:ALA:HB3	2.33	0.58
1:B:49:SER:HB2	1:B:412:GLY:HA2	1.85	0.57
1:B:424:VAL:HB	1:B:431:LEU:HB2	1.87	0.57
1:A:79:PRO:HB2	1:A:83:GLY:HA2	1.87	0.57
1:D:397:ARG:HH12	1:D:449:GLN:HE21	1.52	0.57
1:C:424:VAL:HB	1:C:431:LEU:HB2	1.86	0.57
1:C:382:VAL:O	1:C:391:GLY:HA2	2.05	0.57
1:D:1:ARG:HG2	5:D:2001:HOH:O	2.04	0.56
1:A:78:ALA:HB1	1:A:79:PRO:HD2	1.86	0.56
1:A:150:GLN:HE22	1:A:240:GLU:H	1.52	0.56
1:B:299:ASN:ND2	1:B:302:HIS:H	2.03	0.56
1:A:74:ALA:O	1:A:88:LEU:HD23	2.06	0.56
1:B:203:GLY:N	5:B:2126:HOH:O	2.39	0.56
1:C:11:ALA:O	1:C:14:GLU:HB2	2.06	0.55
1:B:106:MET:O	1:B:110:VAL:HG23	2.07	0.55
1:D:170:SER:HA	1:D:232:VAL:O	2.06	0.55
1:B:45:LEU:HB3	1:B:438:ASN:OD1	2.06	0.55
1:B:226:PRO:HB2	1:B:229:ALA:HB2	1.89	0.55
1:A:292:VAL:HB	1:A:293:PRO:CD	2.36	0.55
1:C:336:VAL:HG22	1:C:366:GLN:HG3	1.87	0.55
1:D:8:ASP:O	1:D:12:ILE:HG13	2.07	0.55
1:A:182:VAL:HG23	1:A:195:ASN:ND2	2.22	0.55
1:D:197:ALA:HB2	1:D:221:VAL:HG12	1.87	0.55
1:A:88:LEU:HD21	1:A:279:LEU:HD12	1.88	0.55
1:D:225:LEU:HD12	1:D:226:PRO:HD2	1.89	0.55
1:D:107:ALA:HB3	1:D:256:ASN:HD22	1.72	0.55
1:C:34:GLU:HB2	5:C:2011:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:GLU:HG3	1:C:201:ALA:HA	1.88	0.54
1:C:47:PRO:O	1:C:50:ASN:HB2	2.07	0.54
1:D:226:PRO:HB2	1:D:229:ALA:HB2	1.89	0.54
1:C:172:THR:HG22	1:C:231:PRO:HB3	1.90	0.54
1:D:2:LEU:HD22	1:D:6:ARG:HE	1.73	0.54
1:A:198:VAL:HG13	1:A:224:SER:HB3	1.89	0.54
1:D:107:ALA:HB3	1:D:256:ASN:ND2	2.23	0.54
1:C:158:HIS:HD2	5:C:2197:HOH:O	1.91	0.54
1:A:321:ASP:O	1:A:325:VAL:HG23	2.07	0.54
1:C:307:VAL:HG11	1:C:324:LEU:HD13	1.90	0.54
1:A:324:LEU:HD12	1:A:343:LEU:HB3	1.89	0.53
1:B:299:ASN:HD22	1:B:299:ASN:C	2.12	0.53
1:A:381:PRO:HD2	1:A:409:ALA:O	2.08	0.53
1:C:73:VAL:HG12	1:C:88:LEU:HD11	1.91	0.53
1:C:78:ALA:HB2	1:C:277:GLU:OE2	2.09	0.53
1:D:381:PRO:O	1:D:408:GLU:HA	2.07	0.53
1:D:28:VAL:HG12	1:D:29:ASP:N	2.23	0.53
1:C:44:GLN:HA	1:C:355:VAL:O	2.09	0.53
1:D:121:ASP:HB2	1:D:123:TYR:CE1	2.44	0.52
1:A:47:PRO:HB3	1:A:355:VAL:CG2	2.39	0.52
1:C:397:ARG:HH12	1:C:449:GLN:HE21	1.56	0.52
1:A:60:LEU:HD21	1:A:291:LEU:HD11	1.91	0.52
1:A:412:GLY:O	1:A:418:SER:HA	2.10	0.52
1:D:150:GLN:HE21	1:D:241:PRO:HD3	1.74	0.52
1:A:60:LEU:HD23	1:A:287:LEU:HD23	1.91	0.52
1:C:125:ASP:CG	1:C:268:GLY:HA2	2.30	0.52
1:D:190:TYR:OH	1:D:243:ALA:HB3	2.10	0.52
1:D:437:ASN:C	1:D:438:ASN:HD22	2.14	0.51
1:A:133:ARG:HB3	1:A:150:GLN:HB3	1.91	0.51
1:B:321:ASP:O	1:B:325:VAL:HG23	2.10	0.51
1:B:397:ARG:NH1	1:B:449:GLN:HE21	2.08	0.51
1:B:119:ARG:NH1	1:B:119:ARG:HG2	2.24	0.51
1:D:296:LYS:HA	1:D:381:PRO:HG3	1.92	0.51
1:A:373:ALA:HB3	5:A:2151:HOH:O	2.09	0.51
1:A:306:LEU:O	1:A:310:ILE:HG13	2.11	0.51
1:A:191:ALA:HA	1:A:217:ASN:ND2	2.26	0.51
1:C:3:THR:O	1:C:7:GLU:HG3	2.11	0.51
1:A:299:ASN:ND2	1:A:302:HIS:H	2.06	0.51
1:A:299:ASN:HB3	1:A:302:HIS:HB2	1.92	0.51
1:B:381:PRO:HD2	1:B:409:ALA:O	2.11	0.51
1:B:300:ASN:OD1	1:B:347:SER:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:GLU:HG2	2:A:504:SO4:O2	2.10	0.51
1:D:94:GLY:O	1:D:96:PRO:HD3	2.11	0.51
1:C:394:LEU:CD1	1:C:411:THR:HG23	2.41	0.50
1:A:292:VAL:HB	1:A:293:PRO:HD3	1.92	0.50
1:C:91:VAL:HG22	1:C:125:ASP:HB3	1.92	0.50
1:A:186:ALA:HB1	1:A:248:LEU:HD11	1.93	0.50
1:A:248:LEU:HD23	1:A:251:GLU:OE2	2.10	0.50
1:B:427:PRO:HG2	1:B:428:GLU:H	1.76	0.50
1:D:184:LEU:HD11	1:D:193:LEU:HD13	1.93	0.50
1:A:198:VAL:HG22	1:A:199:THR:H	1.74	0.50
1:C:312:GLN:O	1:C:316:GLY:HA2	2.12	0.50
1:C:323:GLY:O	1:C:327:VAL:HG23	2.12	0.50
1:C:454:VAL:O	1:C:458:GLU:HG3	2.11	0.50
1:D:100:ALA:O	1:D:103:LEU:HB2	2.12	0.50
1:A:119:ARG:HD2	1:A:261:LYS:HG3	1.93	0.50
1:A:437:ASN:C	1:A:438:ASN:HD22	2.15	0.50
1:A:140:PRO:HG2	1:A:141:GLU:OE1	2.12	0.50
1:A:91:VAL:HG22	1:A:125:ASP:HB3	1.93	0.50
1:A:62:VAL:HG21	1:A:310:ILE:HG23	1.94	0.50
1:A:253:LEU:HB3	1:A:258:VAL:HB	1.94	0.50
1:C:82:ARG:HD3	1:C:84:GLU:OE2	2.11	0.50
1:C:270:PRO:O	1:C:271:ALA:HB3	2.12	0.49
1:B:381:PRO:HB2	1:B:394:LEU:HD12	1.94	0.49
1:C:435:ILE:HD13	1:C:452:ILE:HD12	1.93	0.49
1:A:105:ALA:O	1:A:109:GLU:HG3	2.11	0.49
1:C:286:GLU:HG3	5:C:2153:HOH:O	2.12	0.49
1:A:345:ASP:OD1	1:A:345:ASP:C	2.51	0.49
1:B:46:LEU:HD23	1:B:414:MET:HE3	1.93	0.49
1:A:414:MET:HG3	4:A:520:NCF:H15	1.93	0.49
1:A:423:TYR:HA	1:A:431:LEU:O	2.12	0.49
1:B:288:SER:CB	1:B:375:THR:HG21	2.42	0.49
1:C:263:ASP:HA	5:C:2140:HOH:O	2.12	0.49
1:B:51:MET:HE2	1:B:353:ASN:HB3	1.93	0.49
1:C:129:PHE:CB	1:C:153:ALA:HB2	2.42	0.49
1:B:133:ARG:HG3	1:B:150:GLN:NE2	2.28	0.49
1:D:88:LEU:HD21	1:D:279:LEU:HD12	1.95	0.49
1:D:270:PRO:O	1:D:271:ALA:HB3	2.11	0.49
1:C:28:VAL:HG13	1:C:34:GLU:O	2.12	0.48
1:B:60:LEU:HD13	1:B:372:TRP:CE3	2.48	0.48
1:A:428:GLU:HB2	1:A:460:ALA:C	2.32	0.48
1:D:270:PRO:HB2	1:D:273:TRP:CD1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:ASP:OD2	1:B:284:SER:HB3	2.13	0.48
1:B:9:ILE:HB	1:B:37:TYR:CE2	2.48	0.48
1:C:120:GLY:O	1:C:262:GLY:HA3	2.14	0.48
1:A:226:PRO:HG2	1:A:229:ALA:CB	2.19	0.48
1:D:121:ASP:HB2	1:D:123:TYR:HE1	1.79	0.48
1:B:247:HIS:O	1:B:251:GLU:HG3	2.13	0.48
1:B:270:PRO:O	1:B:271:ALA:HB3	2.14	0.48
1:B:48:ALA:O	1:B:348:GLY:HA3	2.14	0.48
1:B:44:GLN:HA	1:B:355:VAL:O	2.12	0.48
1:D:175:ALA:HB3	1:D:178:GLU:OE1	2.14	0.48
1:C:427:PRO:HA	1:D:112:ALA:HB1	1.94	0.48
1:D:135:VAL:HB	1:D:138:TRP:CD1	2.49	0.48
1:B:343:LEU:HD12	1:B:343:LEU:H	1.77	0.48
1:C:214:VAL:O	1:C:216:THR:HG23	2.13	0.48
1:B:12:ILE:HD13	1:B:451:ALA:HB1	1.96	0.48
1:B:7:GLU:HA	1:B:10:ASP:HB2	1.95	0.48
1:D:270:PRO:HG2	1:D:273:TRP:CE2	2.49	0.48
1:A:9:ILE:HD12	1:A:37:TYR:CD2	2.49	0.48
1:A:137:ASP:OD1	1:A:350:SER:OG	2.32	0.48
1:C:80:GLY:C	1:C:82:ARG:H	2.16	0.47
1:C:321:ASP:O	1:C:325:VAL:HG23	2.13	0.47
1:A:151:ILE:HG22	5:A:2127:HOH:O	2.13	0.47
1:A:397:ARG:HH12	1:A:449:GLN:NE2	2.09	0.47
1:D:138:TRP:CZ2	1:D:349:LEU:HD12	2.49	0.47
1:B:92:GLY:CA	1:B:154:LEU:HG	2.43	0.47
1:D:414:MET:HB3	1:D:417:VAL:HB	1.96	0.47
1:B:130:ASP:OD2	1:B:319:THR:HG22	2.14	0.47
1:D:307:VAL:HG12	1:D:323:GLY:HA3	1.95	0.47
1:B:292:VAL:HB	1:B:293:PRO:CD	2.44	0.47
1:C:63:LEU:O	1:C:67:HIS:HB2	2.13	0.47
1:D:303:ALA:O	1:D:307:VAL:HG23	2.14	0.47
1:C:133:ARG:HB3	1:C:150:GLN:HB3	1.96	0.47
1:A:21:ALA:HB2	1:A:440:HIS:CA	2.45	0.47
1:A:320:TRP:O	1:A:324:LEU:HD23	2.14	0.47
1:A:71:THR:O	1:A:72:GLU:OE2	2.32	0.47
1:D:381:PRO:HB3	1:D:391:GLY:O	2.15	0.47
1:A:154:LEU:HD11	1:A:245:ALA:HB3	1.96	0.47
1:A:103:LEU:HA	1:A:106:MET:HE3	1.97	0.47
1:A:154:LEU:HD13	1:A:245:ALA:HB3	1.97	0.47
1:A:313:GLU:HG3	5:A:2132:HOH:O	2.14	0.46
1:A:29:ASP:HA	1:A:431:LEU:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:VAL:HG12	1:A:237:THR:HA	1.96	0.46
1:A:132:GLU:HG2	1:A:320:TRP:HZ3	1.81	0.46
1:B:133:ARG:HB3	1:B:150:GLN:HB3	1.97	0.46
1:B:360:VAL:O	1:B:364:LEU:HG	2.15	0.46
1:C:184:LEU:HD21	1:C:193:LEU:HD13	1.97	0.46
1:B:202:ALA:HA	1:B:228:ASP:OD1	2.15	0.46
1:A:119:ARG:NH1	1:A:261:LYS:HE3	2.30	0.46
1:A:291:LEU:O	1:A:294:PHE:HB3	2.16	0.46
1:B:410:LYS:NZ	1:B:411:THR:O	2.47	0.46
1:D:76:GLU:OE2	1:D:76:GLU:HA	2.15	0.46
1:C:164:THR:O	1:C:166:VAL:HG13	2.16	0.46
1:A:382:VAL:O	1:A:391:GLY:HA2	2.15	0.46
1:A:298:SER:N	5:A:2125:HOH:O	2.49	0.46
1:D:82:ARG:HD3	1:D:82:ARG:N	2.31	0.46
1:D:3:THR:O	1:D:7:GLU:HG3	2.15	0.46
1:C:381:PRO:CB	1:C:394:LEU:HD13	2.44	0.45
1:B:69:PHE:HA	5:B:2030:HOH:O	2.15	0.45
1:C:171:VAL:HG11	1:C:208:LEU:HD21	1.99	0.45
1:C:129:PHE:CG	1:C:153:ALA:HB2	2.51	0.45
1:C:234:ALA:HB1	1:C:236:ARG:HH12	1.81	0.45
1:D:119:ARG:NH1	1:D:261:LYS:HE3	2.32	0.45
1:C:89:TYR:CZ	1:C:270:PRO:HD3	2.52	0.45
1:D:299:ASN:ND2	1:D:302:HIS:H	2.14	0.45
1:A:392:GLY:O	1:A:394:LEU:N	2.50	0.45
1:B:286:GLU:HG2	5:B:2163:HOH:O	2.16	0.45
1:D:397:ARG:HH12	1:D:449:GLN:NE2	2.13	0.45
1:D:413:THR:HG23	4:D:520:NCF:O4A	2.17	0.45
1:B:403:ALA:HB2	1:B:454:VAL:HA	1.98	0.45
1:C:170:SER:HB2	1:C:183:ASP:HB3	1.99	0.45
1:D:253:LEU:HB3	1:D:258:VAL:HB	1.99	0.45
1:B:270:PRO:HB2	1:B:273:TRP:CD1	2.52	0.45
1:B:361:VAL:HA	1:B:364:LEU:HD12	1.98	0.44
1:B:54:PHE:HB3	1:B:331:LEU:HD11	1.99	0.44
1:B:52:LYS:HD3	1:B:294:PHE:CE2	2.52	0.44
1:B:323:GLY:O	1:B:327:VAL:HG23	2.17	0.44
1:D:299:ASN:HD22	1:D:302:HIS:H	1.64	0.44
1:A:54:PHE:CD2	1:A:363:LEU:HD22	2.52	0.44
1:A:342:VAL:HB	1:A:354:LEU:HB2	1.99	0.44
1:C:98:LEU:HA	5:C:2049:HOH:O	2.16	0.44
1:B:289:GLU:HG3	5:B:2051:HOH:O	2.16	0.44
1:A:117:THR:HG21	1:A:119:ARG:HH11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:ASP:OD1	1:D:39:ARG:NH2	2.51	0.44
1:B:1:ARG:HD2	1:B:3:THR:OG1	2.17	0.44
1:C:47:PRO:O	1:C:48:ALA:HB3	2.17	0.44
1:D:2:LEU:O	1:D:6:ARG:HG3	2.17	0.44
1:A:392:GLY:C	1:A:394:LEU:H	2.21	0.44
1:B:120:GLY:O	1:B:262:GLY:HA3	2.18	0.44
1:A:320:TRP:O	1:A:324:LEU:CD2	2.66	0.43
1:A:463:GLN:HE21	1:A:463:GLN:HB2	1.65	0.43
1:C:292:VAL:HB	1:C:293:PRO:CD	2.48	0.43
1:A:130:ASP:OD2	1:A:319:THR:HA	2.18	0.43
1:D:225:LEU:HD12	1:D:226:PRO:CD	2.46	0.43
1:C:247:HIS:O	1:C:251:GLU:HG3	2.18	0.43
1:B:41:GLY:HA2	1:B:357:ALA:HB3	2.00	0.43
1:D:91:VAL:HG22	1:D:125:ASP:HB3	1.99	0.43
1:A:145:TYR:N	1:A:145:TYR:CD1	2.86	0.43
1:A:372:TRP:O	1:A:375:THR:HG22	2.18	0.43
1:B:384:GLY:HA2	1:B:399:ARG:HG2	2.00	0.43
1:C:291:LEU:O	1:C:379:SER:HB2	2.19	0.43
1:C:320:TRP:O	1:C:324:LEU:HD22	2.19	0.43
1:C:74:ALA:O	1:C:88:LEU:HD12	2.18	0.43
1:B:374:GLN:OE1	1:B:375:THR:HG23	2.19	0.43
1:D:271:ALA:C	1:D:273:TRP:H	2.20	0.43
1:B:342:VAL:HB	1:B:354:LEU:HB2	1.99	0.43
1:C:51:MET:CE	1:C:353:ASN:HB3	2.45	0.43
1:B:335:GLY:HA3	1:B:366:GLN:HE21	1.83	0.43
1:C:54:PHE:HB3	1:C:331:LEU:HD11	2.00	0.43
1:B:385:GLU:O	1:B:391:GLY:HA3	2.19	0.43
1:D:28:VAL:CG1	1:D:29:ASP:N	2.82	0.42
1:A:21:ALA:HB2	1:A:440:HIS:N	2.34	0.42
1:A:54:PHE:HB3	1:A:331:LEU:HD11	2.01	0.42
1:D:47:PRO:O	1:D:48:ALA:HB3	2.18	0.42
1:C:27:VAL:HG12	1:C:36:LEU:HD12	2.01	0.42
1:C:52:LYS:HD3	1:C:294:PHE:CE2	2.54	0.42
1:B:437:ASN:C	1:B:438:ASN:HD22	2.22	0.42
1:A:47:PRO:HB3	1:A:355:VAL:HG21	2.00	0.42
1:D:114:GLY:O	1:D:115:VAL:C	2.57	0.42
1:B:430:GLU:HG2	5:B:2010:HOH:O	2.19	0.42
1:B:98:LEU:HD23	1:B:102:ASP:HB2	2.01	0.42
1:A:122:LEU:HD23	1:A:250:GLU:HB2	2.01	0.42
1:B:29:ASP:O	1:B:33:GLY:N	2.53	0.42
1:A:47:PRO:HB3	1:A:355:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ILE:HB	1:A:37:TYR:CE2	2.54	0.42
1:A:25:VAL:HA	1:A:434:SER:O	2.20	0.42
1:A:271:ALA:HA	5:A:2115:HOH:O	2.20	0.42
1:A:270:PRO:O	1:A:271:ALA:HB3	2.19	0.42
1:C:239:ASP:O	1:C:240:GLU:HB2	2.20	0.42
1:D:82:ARG:HD3	1:D:82:ARG:H	1.83	0.42
1:C:130:ASP:HB2	1:C:318:GLY:O	2.19	0.42
1:D:171:VAL:HG22	1:D:182:VAL:HG22	2.02	0.42
1:B:150:GLN:NE2	1:B:240:GLU:H	2.17	0.42
1:C:139:TRP:HA	1:C:140:PRO:HD3	1.90	0.42
1:C:147:TYR:CD2	4:C:520:NCF:H15	2.55	0.42
1:A:296:LYS:O	1:A:393:THR:HG23	2.20	0.42
1:D:454:VAL:O	1:D:458:GLU:HG3	2.19	0.42
1:D:111:ALA:HB2	1:D:258:VAL:HG23	2.02	0.42
1:B:116:ARG:HH21	1:B:116:ARG:HB3	1.85	0.42
1:C:174:ALA:O	1:C:199:THR:HG21	2.20	0.42
1:B:270:PRO:HG2	1:B:273:TRP:CE2	2.55	0.42
1:C:160:GLU:HG2	2:C:504:SO4:O1	2.19	0.42
1:D:145:TYR:CD1	1:D:145:TYR:N	2.88	0.41
1:B:288:SER:HB2	1:B:375:THR:CG2	2.47	0.41
1:D:397:ARG:NH1	1:D:449:GLN:HE21	2.16	0.41
1:C:94:GLY:O	1:C:96:PRO:HD3	2.19	0.41
1:B:225:LEU:HA	1:B:226:PRO:HD3	1.93	0.41
1:A:171:VAL:HG21	1:A:208:LEU:HD21	2.02	0.41
1:D:341:LEU:HG	1:D:359:THR:HG21	2.02	0.41
1:B:116:ARG:NH2	1:B:116:ARG:HB3	2.36	0.41
1:D:106:MET:O	1:D:110:VAL:HG23	2.19	0.41
1:B:306:LEU:HD23	1:B:306:LEU:HA	1.85	0.41
1:A:198:VAL:HG12	1:A:224:SER:HB3	2.02	0.41
1:A:78:ALA:HB2	1:A:277:GLU:HG2	2.03	0.41
1:A:430:GLU:O	1:A:431:LEU:HD12	2.20	0.41
1:A:63:LEU:HB3	1:A:67:HIS:CG	2.56	0.41
1:C:457:ALA:O	1:C:462:HIS:HB2	2.21	0.41
1:C:4:GLU:HG2	1:C:8:ASP:OD2	2.21	0.41
1:C:270:PRO:C	1:C:272:ASP:N	2.72	0.41
1:D:413:THR:HG22	5:D:2188:HOH:O	2.21	0.41
1:C:86:GLN:HB3	5:C:2038:HOH:O	2.20	0.41
1:D:269:VAL:HB	5:D:2127:HOH:O	2.20	0.41
1:A:121:ASP:HB2	1:A:123:TYR:CE1	2.56	0.41
1:D:9:ILE:HB	1:D:37:TYR:CE2	2.54	0.41
1:B:3:THR:HB	5:B:2001:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:VAL:HG22	1:C:199:THR:H	1.85	0.41
1:B:308:LYS:O	1:B:318:GLY:HA2	2.20	0.41
1:A:81:ARG:C	1:A:83:GLY:H	2.24	0.41
1:D:381:PRO:HD2	1:D:409:ALA:O	2.21	0.41
1:C:234:ALA:HB1	1:C:236:ARG:NH1	2.36	0.41
1:C:135:VAL:HB	1:C:138:TRP:CD1	2.55	0.41
1:D:274:GLN:HA	5:D:2130:HOH:O	2.19	0.41
1:A:336:VAL:O	1:A:338:THR:HG23	2.20	0.41
1:C:136:ASP:OD1	1:C:137:ASP:N	2.54	0.41
1:A:457:ALA:O	1:A:462:HIS:HB2	2.20	0.41
1:C:345:ASP:C	1:C:345:ASP:OD1	2.59	0.41
1:A:173:PRO:HG3	1:A:225:LEU:HD23	2.03	0.41
1:A:314:THR:HA	5:A:2132:HOH:O	2.21	0.40
1:D:158:HIS:HD2	5:D:2084:HOH:O	2.04	0.40
1:A:380:LEU:HA	1:A:381:PRO:HD3	1.92	0.40
1:D:184:LEU:HD13	1:D:193:LEU:HD22	2.04	0.40
1:C:409:ALA:HA	1:C:422:GLY:HA3	2.04	0.40
1:A:214:VAL:HG12	5:A:2101:HOH:O	2.20	0.40
1:B:376:TRP:HE1	1:B:423:TYR:HE2	1.69	0.40
1:C:37:TYR:CD1	1:C:38:SER:N	2.89	0.40
1:B:399:ARG:NH1	5:B:2196:HOH:O	2.54	0.40
1:B:341:LEU:HG	1:B:359:THR:HG21	2.03	0.40
1:A:212:ARG:O	1:A:213:PRO:C	2.60	0.40
1:D:348:GLY:HA2	1:D:353:ASN:ND2	2.36	0.40
1:C:61:GLU:OE1	1:C:334:LEU:HD13	2.20	0.40
1:D:287:LEU:O	1:D:291:LEU:HB2	2.22	0.40
1:D:5:LEU:O	1:D:9:ILE:HG13	2.21	0.40
1:B:110:VAL:HG12	1:B:115:VAL:HB	2.02	0.40
1:D:341:LEU:CD2	1:D:355:VAL:HG12	2.51	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	465/489 (95%)	423 (91%)	39 (8%)	3 (1%)	30	43
1	B	464/489 (95%)	430 (93%)	32 (7%)	2 (0%)	39	56
1	C	464/489 (95%)	434 (94%)	30 (6%)	0	100	100
1	D	465/489 (95%)	430 (92%)	32 (7%)	3 (1%)	30	43
All	All	1858/1956 (95%)	1717 (92%)	133 (7%)	8 (0%)	39	56

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	ARG
1	A	393	THR
1	D	86	GLN
1	A	270	PRO
1	B	270	PRO
1	B	374	GLN
1	D	279	LEU
1	D	115	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	339/356 (95%)	328 (97%)	11 (3%)	46	68
1	B	338/356 (95%)	323 (96%)	15 (4%)	35	53
1	C	338/356 (95%)	325 (96%)	13 (4%)	40	60
1	D	339/356 (95%)	324 (96%)	15 (4%)	35	53
All	All	1354/1424 (95%)	1300 (96%)	54 (4%)	38	58

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	141	GLU
1	A	183	ASP

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Mol	Chain	Res	Type
1	A	216	THR
1	A	250	GLU
1	A	299	ASN
1	A	312	GLN
1	A	320	TRP
1	A	376	TRP
1	A	455	ARG
1	A	463	GLN
1	B	8	ASP
1	B	10	ASP
1	B	18	LEU
1	B	43	GLU
1	B	88	LEU
1	B	98	LEU
1	B	154	LEU
1	B	198	VAL
1	B	270	PRO
1	B	274	GLN
1	B	299	ASN
1	B	320	TRP
1	B	324	LEU
1	B	349	LEU
1	B	463	GLN
1	C	19	GLU
1	C	50	ASN
1	C	72	GLU
1	C	134	LEU
1	C	154	LEU
1	C	272	ASP
1	C	299	ASN
1	C	302	HIS
1	C	320	TRP
1	C	324	LEU
1	C	349	LEU
1	C	376	TRP
1	C	438	ASN
1	D	2	LEU
1	D	46	LEU
1	D	63	LEU
1	D	82	ARG
1	D	88	LEU
1	D	98	LEU

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Mol	Chain	Res	Type
1	D	154	LEU
1	D	183	ASP
1	D	196	ARG
1	D	291	LEU
1	D	299	ASN
1	D	320	TRP
1	D	324	LEU
1	D	374	GLN
1	D	413	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	150	GLN
1	A	158	HIS
1	A	299	ASN
1	A	312	GLN
1	A	437	ASN
1	A	449	GLN
1	A	463	GLN
1	B	44	GLN
1	B	50	ASN
1	B	150	GLN
1	B	299	ASN
1	B	302	HIS
1	B	366	GLN
1	B	396	ASN
1	B	437	ASN
1	B	449	GLN
1	B	463	GLN
1	C	50	ASN
1	C	158	HIS
1	C	256	ASN
1	C	299	ASN
1	C	366	GLN
1	C	437	ASN
1	C	449	GLN
1	D	50	ASN
1	D	150	GLN
1	D	158	HIS
1	D	256	ASN

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Mol	Chain	Res	Type
1	D	299	ASN
1	D	437	ASN
1	D	449	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 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	501	-	4,4,4	0.29	0	6,6,6	0.15	0
2	SO4	A	502	-	4,4,4	0.33	0	6,6,6	0.18	0
2	SO4	A	503	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	A	504	-	4,4,4	0.34	0	6,6,6	0.07	0
4	NCF	A	520	1	14,22,22	2.26	3 (21%)	8,29,29	2.49	2 (25%)
2	SO4	B	501	-	4,4,4	0.20	0	6,6,6	0.11	0
2	SO4	B	502	-	4,4,4	0.29	0	6,6,6	0.08	0
2	SO4	B	503	-	4,4,4	0.31	0	6,6,6	0.05	0
2	SO4	B	504	-	4,4,4	0.32	0	6,6,6	0.19	0
4	NCF	B	520	1	14,22,22	2.44	3 (21%)	8,29,29	2.79	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	C	501	-	4,4,4	0.23	0	6,6,6	0.11	0
2	SO4	C	502	-	4,4,4	0.27	0	6,6,6	0.14	0
2	SO4	C	503	-	4,4,4	0.30	0	6,6,6	0.09	0
2	SO4	C	504	-	4,4,4	0.23	0	6,6,6	0.17	0
4	NCF	C	520	1	14,22,22	2.70	3 (21%)	8,29,29	2.78	2 (25%)
2	SO4	D	501	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	D	502	-	4,4,4	0.31	0	6,6,6	0.10	0
2	SO4	D	503	-	4,4,4	0.24	0	6,6,6	0.12	0
2	SO4	D	504	-	4,4,4	0.31	0	6,6,6	0.11	0
4	NCF	D	520	1	14,22,22	2.56	4 (28%)	8,29,29	2.68	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	501	-	-	0/0/0/0	0/0/0/0
2	SO4	A	502	-	-	0/0/0/0	0/0/0/0
2	SO4	A	503	-	-	0/0/0/0	0/0/0/0
2	SO4	A	504	-	-	0/0/0/0	0/0/0/0
4	NCF	A	520	1	-	0/6/28/28	0/1/2/2
2	SO4	B	501	-	-	0/0/0/0	0/0/0/0
2	SO4	B	502	-	-	0/0/0/0	0/0/0/0
2	SO4	B	503	-	-	0/0/0/0	0/0/0/0
2	SO4	B	504	-	-	0/0/0/0	0/0/0/0
4	NCF	B	520	1	-	0/6/28/28	0/1/2/2
2	SO4	C	501	-	-	0/0/0/0	0/0/0/0
2	SO4	C	502	-	-	0/0/0/0	0/0/0/0
2	SO4	C	503	-	-	0/0/0/0	0/0/0/0
2	SO4	C	504	-	-	0/0/0/0	0/0/0/0
4	NCF	C	520	1	-	0/6/28/28	0/1/2/2
2	SO4	D	501	-	-	0/0/0/0	0/0/0/0
2	SO4	D	502	-	-	0/0/0/0	0/0/0/0
2	SO4	D	503	-	-	0/0/0/0	0/0/0/0
2	SO4	D	504	-	-	0/0/0/0	0/0/0/0
4	NCF	D	520	1	-	0/6/28/28	0/1/2/2

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	520	NCF	C13-C14	-3.95	1.48	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	520	NCF	C3-C4	3.03	1.53	1.50
4	D	520	NCF	C7-N10	3.46	1.50	1.46
4	A	520	NCF	C3-C4	3.56	1.54	1.50
4	C	520	NCF	C3-C4	3.78	1.54	1.50
4	A	520	NCF	C7-N10	3.80	1.50	1.46
4	D	520	NCF	C3-C4	4.35	1.54	1.50
4	B	520	NCF	C7-N10	4.81	1.51	1.46
4	D	520	NCF	C11-N10	5.78	1.45	1.34
4	C	520	NCF	C7-N10	5.84	1.52	1.46
4	A	520	NCF	C11-N10	5.85	1.45	1.34
4	B	520	NCF	C11-N10	6.34	1.46	1.34
4	C	520	NCF	C11-N10	6.68	1.47	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	520	NCF	C16-C17-S19	-3.78	109.04	113.23
4	B	520	NCF	C16-C17-S19	-3.45	109.41	113.23
4	D	520	NCF	C16-C17-S19	-3.39	109.47	113.23
4	A	520	NCF	C16-C17-S19	-3.23	109.66	113.23
4	A	520	NCF	C3-C2-S1	5.65	119.51	112.99
4	D	520	NCF	C3-C2-S1	6.24	120.18	112.99
4	C	520	NCF	C3-C2-S1	6.45	120.43	112.99
4	B	520	NCF	C3-C2-S1	6.68	120.69	112.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	SO4	1	0
2	A	504	SO4	1	0
4	A	520	NCF	1	0
2	C	504	SO4	1	0
4	C	520	NCF	1	0
4	D	520	NCF	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	467/489 (95%)	0.48	37 (7%)	15	15	24, 46, 67, 82	0
1	B	466/489 (95%)	0.13	15 (3%)	51	51	21, 42, 66, 83	0
1	C	466/489 (95%)	0.11	19 (4%)	41	42	21, 43, 65, 81	0
1	D	467/489 (95%)	0.17	19 (4%)	41	42	19, 34, 68, 81	0
All	All	1866/1956 (95%)	0.22	90 (4%)	34	35	19, 42, 67, 83	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	466	GLU	7.9
1	A	279	LEU	5.8
1	D	82	ARG	5.1
1	A	73	VAL	5.0
1	A	110	VAL	4.9
1	D	260	VAL	4.4
1	A	81	ARG	4.4
1	D	262	GLY	4.3
1	D	119	ARG	4.2
1	C	83	GLY	4.0
1	C	82	ARG	4.0
1	D	264	VAL	3.9
1	B	2	LEU	3.8
1	D	429	GLY	3.6
1	C	81	ARG	3.6
1	A	108	ALA	3.6
1	B	274	GLN	3.5
1	A	111	ALA	3.5
1	A	78	ALA	3.4
1	A	275	ASP	3.3
1	A	83	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	374	GLN	3.3
1	A	77	SER	3.2
1	C	429	GLY	3.2
1	A	82	ARG	3.2
1	A	253	LEU	3.2
1	C	6	ARG	3.1
1	B	32	THR	3.1
1	C	371	PRO	3.1
1	D	115	VAL	3.1
1	A	272	ASP	3.1
1	D	275	ASP	3.1
1	A	260	VAL	3.1
1	A	255	SER	3.0
1	B	31	ALA	3.0
1	D	257	GLY	3.0
1	A	2	LEU	3.0
1	A	91	VAL	2.9
1	C	314	THR	2.9
1	A	115	VAL	2.9
1	A	117	THR	2.9
1	B	428	GLU	2.9
1	C	117	THR	2.8
1	A	116	ARG	2.8
1	D	77	SER	2.8
1	B	461	GLY	2.8
1	C	1	ARG	2.7
1	B	425	PRO	2.7
1	A	280	ALA	2.7
1	A	80	GLY	2.7
1	C	7	GLU	2.7
1	A	106	MET	2.6
1	A	264	VAL	2.6
1	A	156	VAL	2.6
1	C	428	GLU	2.6
1	D	79	PRO	2.6
1	A	371	PRO	2.5
1	C	4	GLU	2.5
1	D	31	ALA	2.5
1	D	276	ALA	2.5
1	C	2	LEU	2.5
1	A	114	GLY	2.5
1	C	375	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	104	ASP	2.4
1	B	3	THR	2.4
1	D	110	VAL	2.4
1	D	118	VAL	2.4
1	A	71	THR	2.4
1	C	259	THR	2.4
1	D	83	GLY	2.4
1	A	88	LEU	2.4
1	B	262	GLY	2.3
1	A	254	GLU	2.3
1	A	282	HIS	2.3
1	B	463	GLN	2.3
1	B	317	ALA	2.3
1	A	6	ARG	2.2
1	A	269	VAL	2.2
1	A	262	GLY	2.2
1	A	276	ALA	2.2
1	C	11	ALA	2.2
1	B	271	ALA	2.2
1	A	32	THR	2.1
1	C	84	GLU	2.1
1	C	119	ARG	2.0
1	D	81	ARG	2.0
1	B	35	GLU	2.0
1	D	258	VAL	2.0
1	B	464	ALA	2.0
1	D	259	THR	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MG	D	511	1/1	0.99	0.22	3.20	12,12,12,12	0
3	MG	D	510	1/1	0.98	0.20	2.04	21,21,21,21	0
2	SO4	B	504	5/5	0.89	0.22	1.92	75,76,78,78	0
2	SO4	C	504	5/5	0.96	0.17	1.53	74,75,75,76	0
4	NCF	D	520	21/21	0.93	0.24	1.49	27,32,41,45	0
3	MG	A	511	1/1	0.99	0.21	1.09	24,24,24,24	0
4	NCF	A	520	21/21	0.90	0.24	1.06	31,37,44,49	0
4	NCF	C	520	21/21	0.88	0.18	0.76	35,44,48,51	0
4	NCF	B	520	21/21	0.94	0.19	-0.00	35,41,45,49	0
3	MG	A	510	1/1	0.98	0.17	-0.39	28,28,28,28	0
2	SO4	D	504	5/5	0.94	0.12	-1.83	73,74,74,75	0
2	SO4	C	501	5/5	0.95	0.13	-	65,65,66,66	0
2	SO4	A	501	5/5	0.94	0.17	-	67,67,69,70	0
2	SO4	C	502	5/5	0.98	0.10	-	61,61,62,63	0
2	SO4	B	503	5/5	0.99	0.13	-	59,59,61,61	0
2	SO4	A	502	5/5	0.88	0.20	-	74,75,75,76	0
2	SO4	D	503	5/5	0.97	0.18	-	55,56,57,59	0
2	SO4	A	503	5/5	0.97	0.12	-	73,73,74,74	0
2	SO4	B	502	5/5	0.95	0.11	-	75,75,76,77	0
2	SO4	A	504	5/5	0.93	0.13	-	80,81,81,82	0
2	SO4	D	502	5/5	0.84	0.23	-	79,80,82,82	0
2	SO4	D	501	5/5	0.96	0.11	-	62,63,64,65	0
2	SO4	B	501	5/5	0.98	0.14	-	69,70,70,70	0
2	SO4	C	503	5/5	0.97	0.14	-	56,57,57,58	0

6.5 Other polymers (i)

There are no such residues in this entry.