Full wwPDB X-ray Structure Validation Report (i)

Jan 3, 2024 – 12:23 pm GMT

PDB ID	:	5LHS
Title	:	The ligand free catalytic domain of murine urokinase-type plasminogen activator
Authors	:	Kromann-Hansen, T.; Lange, E.L.; Sorensen, H.P.; Ghassabeh, G.H.; Huang, M.; Jensen, J.K.; Muyldermans, S.; Declerck, P.J.; Andreasen, P.A.
Deposited on	:	2016-07-12
Resolution	:	3.05 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

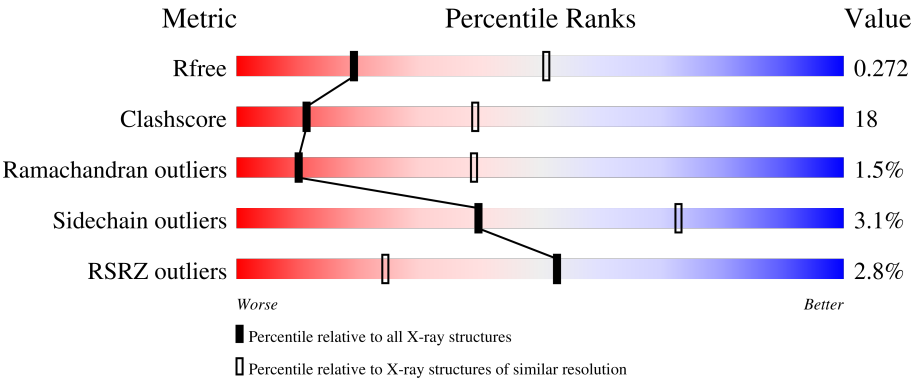
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.05 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}	130704	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	247	2% 61% 26% 9%
1	B	247	3% 63% 25% 9%
1	C	247	3% 65% 22% 9%
1	D	247	2% 65% 23% 9%

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
2	SO4	C	302	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7056 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.

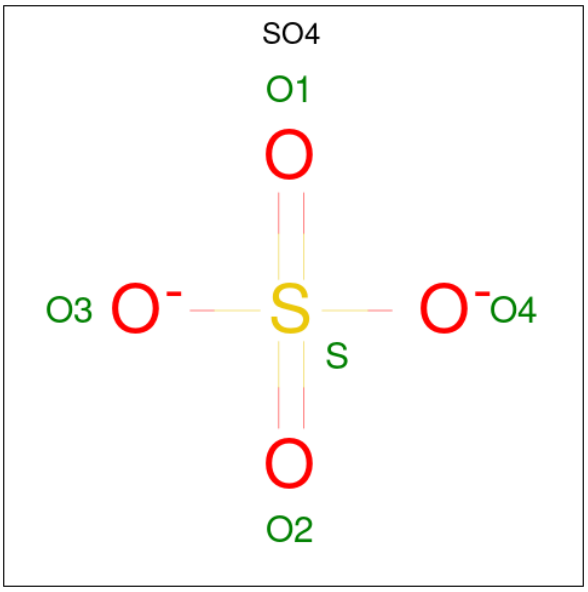
- Molecule 1 is a protein called Urokinase-type plasminogen activator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	224	Total	C	N	O	S	0	0	0
			1753	1118	298	323	14			
1	A	224	Total	C	N	O	S	0	0	0
			1753	1118	298	323	14			
1	C	224	Total	C	N	O	S	0	0	0
			1753	1118	298	323	14			
1	D	224	Total	C	N	O	S	0	0	0
			1753	1118	298	323	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	122	ALA	CYS	engineered mutation	UNP P06869
A	122	ALA	CYS	engineered mutation	UNP P06869
C	122	ALA	CYS	engineered mutation	UNP P06869
D	122	ALA	CYS	engineered mutation	UNP P06869

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



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

- Molecule 3 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

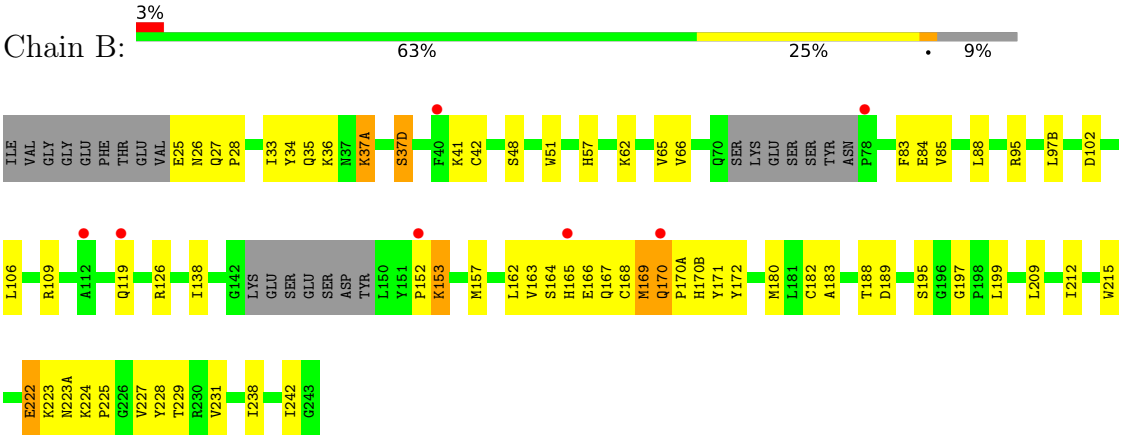
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ni 1 1	0	0
3	A	1	Total Ni 1 1	0	0
3	C	2	Total Ni 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

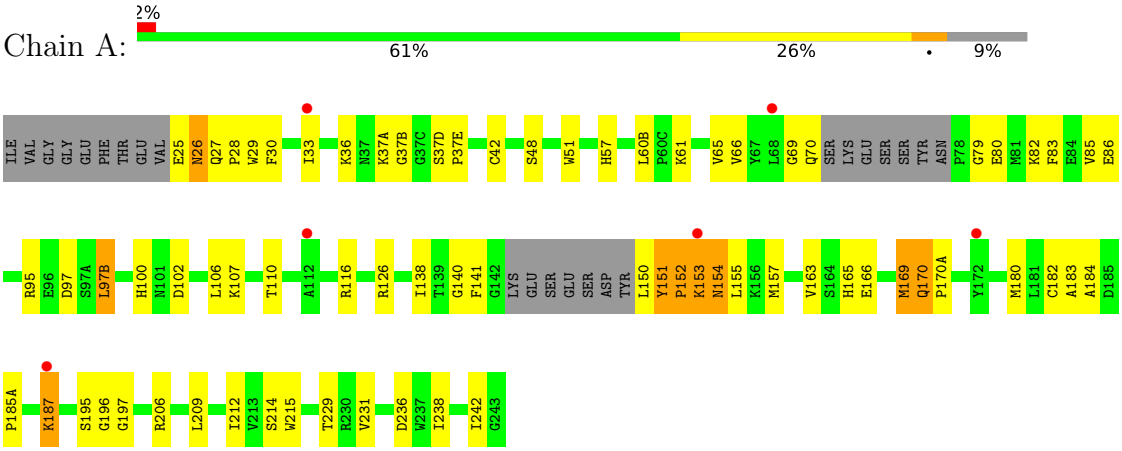
• Molecule 1: Urokinase-type plasminogen activator

Chain B:



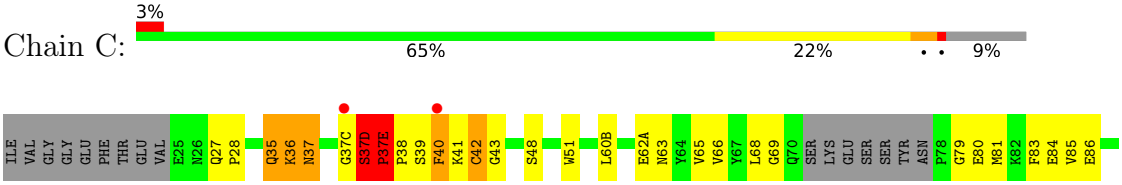
• Molecule 1: Urokinase-type plasminogen activator

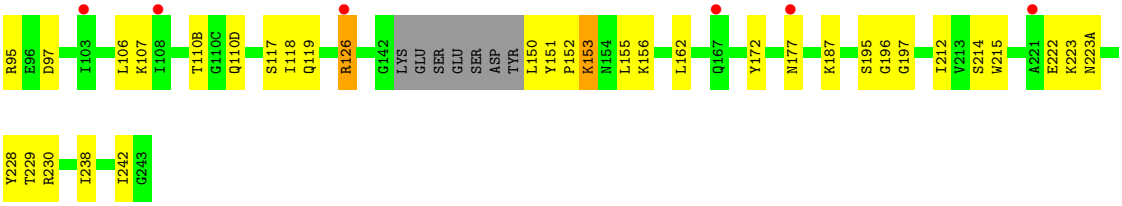
Chain A:



• Molecule 1: Urokinase-type plasminogen activator

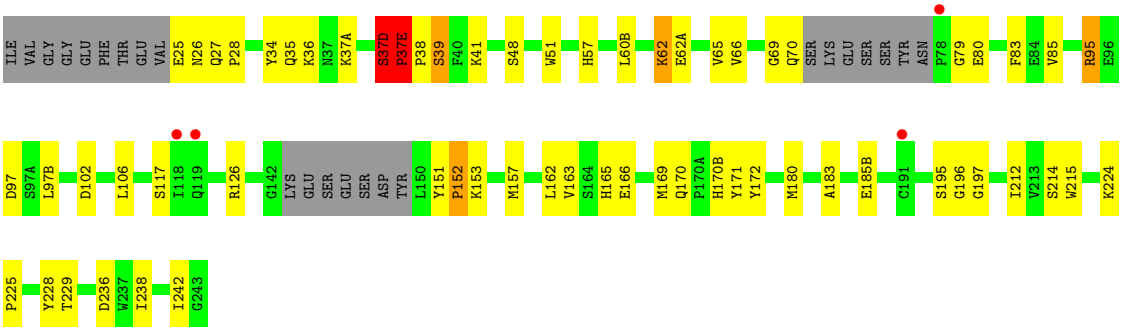
Chain C:





• Molecule 1: Urokinase-type plasminogen activator

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	194.70Å 194.70Å 37.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.68 – 3.05 48.68 – 3.05	Depositor EDS
% Data completeness (in resolution range)	98.4 (38.68-3.05) 98.5 (48.68-3.05)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.86 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.213 , 0.260 0.229 , 0.272	Depositor DCC
R_{free} test set	1476 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	74.8	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.468 for -h,-k,l 0.468 for h,-h-k,-l 0.468 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7056	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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, 0.333 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: NI, 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	0.34	0/1802	0.59	2/2439 (0.1%)
1	B	0.37	0/1802	0.60	1/2439 (0.0%)
1	C	0.40	0/1802	0.64	5/2439 (0.2%)
1	D	0.31	0/1802	0.83	5/2439 (0.2%)
All	All	0.36	0/7208	0.67	13/9756 (0.1%)

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
1	C	0	1
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	37(E)	PRO	CA-C-O	-26.23	57.24	120.20
1	D	37(E)	PRO	CA-C-N	13.62	155.23	117.10
1	D	37(E)	PRO	O-C-N	-12.16	97.99	121.10
1	C	126	ARG	NE-CZ-NH2	-7.43	116.58	120.30
1	C	126	ARG	NE-CZ-NH1	7.29	123.95	120.30
1	A	97(B)	LEU	CB-CG-CD2	6.90	122.72	111.00
1	C	150	LEU	CA-CB-CG	5.99	129.09	115.30
1	A	37(E)	PRO	C-N-CD	5.42	139.78	128.40
1	D	37(D)	SER	C-N-CD	5.17	139.25	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	37(E)	PRO	C-N-CD	5.13	139.18	128.40
1	B	37(D)	SER	C-N-CD	5.09	139.08	128.40
1	C	37(D)	SER	C-N-CD	5.07	139.04	128.40
1	D	37(E)	PRO	C-N-CD	5.06	139.02	128.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	26	ASN	Peptide
1	C	153	LYS	Peptide
1	D	37(E)	PRO	Mainchain

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	1753	0	1695	70	0
1	B	1753	0	1697	64	0
1	C	1753	0	1695	51	0
1	D	1753	0	1695	77	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	1	0
2	D	10	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
All	All	7056	0	6782	243	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 (243) 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:168:CYS:SG	1:B:182:CYS:SG	1.29	1.28
1:D:69:GLY:HA3	1:D:80:GLU:CG	1.67	1.24
1:D:34:TYR:CD2	1:D:39:SER:O	2.07	1.07
1:D:36:LYS:HA	1:D:38:PRO:HG3	1.38	1.06
1:B:170(B):HIS:CD2	1:B:171:TYR:CE1	2.45	1.04
1:C:42:CYS:O	1:C:196:GLY:O	1.74	1.03
1:A:151:TYR:O	1:A:154:ASN:ND2	1.91	1.03
1:D:69:GLY:HA3	1:D:80:GLU:HG2	1.36	1.03
1:D:36:LYS:HA	1:D:38:PRO:CG	1.89	1.02
1:D:34:TYR:HD2	1:D:39:SER:O	1.39	1.01
1:D:62:LYS:H	1:D:62:LYS:HD2	1.25	1.00
1:A:151:TYR:HB3	1:A:152:PRO:HD2	1.51	0.93
1:A:169:MET:CE	1:D:171:TYR:CE2	2.53	0.93
1:D:95:ARG:HH12	1:D:97:ASP:HB3	1.37	0.88
1:C:42:CYS:SG	1:C:196:GLY:N	2.47	0.88
1:A:27:GLN:H	1:A:30:PHE:HB3	1.39	0.87
1:D:36:LYS:HE3	1:D:65:VAL:HG23	1.56	0.87
1:A:151:TYR:CB	1:A:152:PRO:HD2	2.05	0.86
1:A:169:MET:HE3	1:D:171:TYR:CE2	2.10	0.86
1:D:69:GLY:HA3	1:D:80:GLU:HG3	1.56	0.85
1:A:95:ARG:HH22	1:A:185(A):PRO:HB3	1.42	0.84
1:D:70:GLN:O	1:D:79:GLY:HA2	1.79	0.82
1:C:80:GLU:O	1:C:81:MET:HG2	1.80	0.82
1:C:65:VAL:HG22	1:C:84:GLU:HG2	1.63	0.80
1:A:25:GLU:N	1:A:27:GLN:OE1	2.14	0.80
1:A:150:LEU:HB2	1:A:151:TYR:CE1	2.16	0.80
1:A:170:GLN:HE22	1:D:170:GLN:HE22	1.28	0.78
1:B:48:SER:HB3	1:B:51:TRP:HB2	1.64	0.78
1:D:69:GLY:CA	1:D:80:GLU:HG2	2.13	0.78
1:D:48:SER:HB3	1:D:51:TRP:HB2	1.66	0.78
1:B:222:GLU:OE2	1:B:223(A):ASN:N	2.18	0.76
1:A:48:SER:HB3	1:A:51:TRP:HB2	1.66	0.76
1:B:188:THR:HB	1:B:227:VAL:HG21	1.68	0.75
1:B:167:GLN:O	1:B:170(A):PRO:HG3	1.87	0.74
1:A:152:PRO:O	1:A:154:ASN:ND2	2.21	0.74
1:B:36:LYS:NZ	1:B:84:GLU:OE2	2.17	0.74
1:D:70:GLN:H	1:D:80:GLU:HG2	1.54	0.72
1:C:36:LYS:HD2	1:C:62(A):GLU:O	1.90	0.71
1:D:195:SER:HB3	1:D:215:TRP:HB2	1.72	0.71
1:B:195:SER:HB3	1:B:215:TRP:HB2	1.71	0.71
1:C:177:ASN:O	1:C:223:LYS:NZ	2.20	0.71
1:D:70:GLN:N	1:D:80:GLU:HG2	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:GLN:HG3	1:A:28:PRO:HD2	1.73	0.70
1:A:169:MET:HE1	1:D:171:TYR:CE2	2.27	0.69
1:D:35:GLN:HB2	1:D:41:LYS:HG3	1.73	0.69
1:C:110(B):THR:HG23	1:C:110(D):GLN:HG2	1.73	0.69
1:D:35:GLN:NE2	1:D:60(B):LEU:HD12	2.08	0.69
1:B:170(B):HIS:HD2	1:B:171:TYR:CE1	2.07	0.69
1:B:37(A):LYS:HD3	1:B:37(A):LYS:H	1.58	0.68
1:C:48:SER:HB3	1:C:51:TRP:HB2	1.75	0.68
1:C:126:ARG:HH12	1:D:95:ARG:HD3	1.58	0.68
1:D:25:GLU:HG2	1:D:26:ASN:H	1.58	0.68
1:A:195:SER:HB3	1:A:215:TRP:HB2	1.76	0.66
1:C:80:GLU:O	1:C:80:GLU:HG2	1.94	0.66
1:C:195:SER:HB3	1:C:215:TRP:HB2	1.78	0.66
1:C:37(D):SER:HB2	1:C:37(E):PRO:CD	2.27	0.64
1:B:166:GLU:OE1	1:B:166:GLU:N	2.30	0.64
1:C:86:GLU:OE1	1:C:107:LYS:NZ	2.30	0.64
1:B:37(A):LYS:HD3	1:B:37(A):LYS:N	2.15	0.62
1:B:169:MET:O	1:B:170:GLN:HB3	2.00	0.62
1:C:238:ILE:O	1:C:242:ILE:HG12	2.00	0.62
1:D:165:HIS:NE2	1:D:183:ALA:O	2.31	0.62
1:A:97(B):LEU:HD22	1:A:187:LYS:HG2	1.82	0.62
1:A:151:TYR:HB3	1:A:152:PRO:CD	2.29	0.61
1:D:95:ARG:NH1	1:D:97:ASP:HB3	2.11	0.61
1:C:37:ASN:HB2	1:C:38:PRO:HA	1.81	0.61
1:A:151:TYR:CB	1:A:152:PRO:CD	2.77	0.61
1:D:37(D):SER:HB3	1:D:37(E):PRO:HD3	1.83	0.61
1:B:170(B):HIS:CD2	1:B:171:TYR:CD1	2.89	0.61
1:D:66:VAL:HG22	1:D:83:PHE:HB2	1.83	0.60
1:C:230:ARG:NH1	1:D:185(B):GLU:OE2	2.35	0.60
1:B:170:GLN:H	1:B:170(A):PRO:HD3	1.66	0.60
1:C:35:GLN:NE2	1:C:60(B):LEU:HD12	2.16	0.60
1:D:126:ARG:NH1	1:D:236:ASP:OD1	2.34	0.60
1:B:170:GLN:O	1:B:170:GLN:HG3	2.02	0.60
1:B:126:ARG:HH12	1:A:97:ASP:CB	2.15	0.59
1:D:69:GLY:CA	1:D:80:GLU:CG	2.61	0.59
1:A:170:GLN:HE22	1:D:170:GLN:NE2	2.00	0.58
1:D:36:LYS:HE3	1:D:65:VAL:CG2	2.30	0.58
1:C:80:GLU:OE1	1:C:117:SER:OG	2.21	0.58
1:D:35:GLN:C	1:D:38:PRO:HB3	2.23	0.58
1:D:238:ILE:O	1:D:242:ILE:HG12	2.04	0.58
1:B:170:GLN:HA	1:B:170(B):HIS:CE1	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:GLU:OE2	1:C:223(A):ASN:N	2.33	0.57
1:D:35:GLN:O	1:D:38:PRO:HB3	2.04	0.57
1:D:80:GLU:OE1	1:D:117:SER:HB2	2.04	0.57
1:A:150:LEU:HB2	1:A:151:TYR:CD1	2.39	0.57
1:A:238:ILE:O	1:A:242:ILE:HG12	2.04	0.57
1:C:42:CYS:SG	1:C:196:GLY:CA	2.92	0.57
1:B:126:ARG:HH12	1:A:97:ASP:HB3	1.69	0.57
1:B:26:ASN:HB2	1:B:153:LYS:HZ1	1.68	0.57
1:B:238:ILE:O	1:B:242:ILE:HG12	2.04	0.57
1:A:27:GLN:HG2	1:A:29:TRP:CE2	2.39	0.57
1:C:151:TYR:HB3	1:C:152:PRO:HD2	1.87	0.57
1:D:69:GLY:HA3	1:D:80:GLU:CD	2.25	0.56
1:C:40:PHE:CD1	1:C:41:LYS:N	2.73	0.56
1:B:170:GLN:N	1:B:170(A):PRO:HD3	2.20	0.56
1:D:35:GLN:HB2	1:D:41:LYS:CG	2.35	0.56
1:A:26:ASN:OD1	1:A:27:GLN:HA	2.05	0.56
1:C:37(E):PRO:HB2	1:C:38:PRO:CD	2.36	0.56
1:A:85:VAL:HG11	1:A:106:LEU:HD22	1.88	0.55
1:B:34:TYR:OH	1:B:152:PRO:HG3	2.06	0.55
1:B:212:ILE:HB	1:B:229:THR:HB	1.89	0.55
1:C:36:LYS:N	1:C:63:ASN:O	2.37	0.55
1:A:126:ARG:NH1	1:A:236:ASP:OD1	2.40	0.55
1:A:66:VAL:HG22	1:A:83:PHE:HB2	1.90	0.54
1:C:69:GLY:HA3	1:C:80:GLU:HB3	1.88	0.54
1:C:66:VAL:HG22	1:C:83:PHE:HB2	1.88	0.54
1:C:85:VAL:HG11	1:C:106:LEU:HD22	1.89	0.54
1:A:86:GLU:OE1	1:A:107:LYS:NZ	2.34	0.54
1:D:37(D):SER:CB	1:D:37(E):PRO:CD	2.86	0.53
1:D:170:GLN:HB2	1:D:170(B):HIS:CE1	2.43	0.53
1:A:163:VAL:HG11	1:A:180:MET:HE3	1.90	0.53
1:B:168:CYS:C	1:B:169:MET:HG2	2.28	0.53
1:A:69:GLY:HA3	1:A:80:GLU:HB3	1.89	0.53
1:D:34:TYR:OH	1:D:152:PRO:HG3	2.09	0.53
1:A:95:ARG:NH2	1:A:185(A):PRO:HB3	2.19	0.53
1:B:85:VAL:HG11	1:B:106:LEU:HD22	1.90	0.53
1:A:212:ILE:HB	1:A:229:THR:HB	1.90	0.53
1:B:66:VAL:HG22	1:B:83:PHE:HB2	1.91	0.53
1:C:51:TRP:CG	1:C:242:ILE:HD12	2.44	0.53
1:D:85:VAL:HG11	1:D:106:LEU:HD22	1.90	0.52
1:D:80:GLU:CD	1:D:117:SER:HG	2.13	0.52
1:A:169:MET:O	1:A:170:GLN:HB3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:GLN:HE21	1:D:60(B):LEU:HD12	1.74	0.52
1:D:36:LYS:HD2	1:D:62(A):GLU:O	2.09	0.52
1:B:51:TRP:CG	1:B:242:ILE:HD12	2.45	0.52
1:B:170(B):HIS:NE2	1:B:171:TYR:CE1	2.77	0.52
1:C:95:ARG:CZ	1:D:126:ARG:HD3	2.41	0.51
1:D:151:TYR:O	1:D:153:LYS:N	2.44	0.51
1:D:37(D):SER:HB3	1:D:37(E):PRO:CD	2.40	0.51
1:D:27:GLN:HB3	1:D:28:PRO:HD2	1.92	0.51
1:D:165:HIS:O	1:D:169:MET:HG2	2.11	0.51
1:B:62:LYS:HD3	1:B:88:LEU:HB3	1.93	0.50
1:C:153:LYS:C	1:C:155:LEU:H	2.15	0.50
1:A:27:GLN:HB3	1:A:30:PHE:HB2	1.92	0.50
1:C:40:PHE:CD1	1:C:40:PHE:C	2.84	0.50
1:A:37(A):LYS:HG2	1:A:37(B):GLY:N	2.26	0.50
1:D:36:LYS:CE	1:D:65:VAL:HG23	2.36	0.49
1:D:36:LYS:CD	1:D:62(A):GLU:O	2.61	0.49
1:A:170:GLN:N	1:A:170(A):PRO:HD3	2.28	0.49
1:B:170(B):HIS:HD2	1:B:171:TYR:HE1	1.60	0.49
1:B:95:ARG:CZ	1:A:126:ARG:HD3	2.43	0.49
1:D:166:GLU:OE1	1:D:166:GLU:N	2.46	0.48
1:D:57:HIS:ND1	1:D:102:ASP:OD2	2.47	0.48
1:C:27:GLN:OE1	1:C:27:GLN:N	2.45	0.48
1:D:36:LYS:HA	1:D:38:PRO:CB	2.43	0.48
1:A:155:LEU:HD11	1:A:215:TRP:CZ2	2.48	0.48
1:B:97(B):LEU:HG	1:B:189:ASP:H	1.79	0.48
1:B:165:HIS:NE2	1:B:183:ALA:O	2.38	0.48
1:B:170(B):HIS:NE2	1:B:171:TYR:CZ	2.82	0.47
1:B:152:PRO:O	1:B:153:LYS:HB2	2.13	0.47
1:B:197:GLY:HA3	1:B:215:TRP:CZ2	2.50	0.47
1:A:27:GLN:HG3	1:A:28:PRO:CD	2.43	0.47
1:B:37(A):LYS:N	1:B:37(A):LYS:CD	2.78	0.47
1:D:51:TRP:CG	1:D:242:ILE:HD12	2.50	0.47
1:A:151:TYR:CD1	1:A:151:TYR:N	2.82	0.47
1:C:212:ILE:HB	1:C:229:THR:HB	1.95	0.46
1:C:28:PRO:HB2	1:C:119:GLN:H	1.80	0.46
1:B:172:TYR:OH	1:C:172:TYR:OH	2.08	0.46
1:B:223:LYS:HD3	1:B:223:LYS:N	2.31	0.46
1:A:82:LYS:O	1:A:110:THR:HG22	2.16	0.46
1:A:51:TRP:CG	1:A:242:ILE:HD12	2.50	0.46
1:C:37:ASN:HB2	1:C:37(E):PRO:O	2.14	0.46
1:D:80:GLU:OE1	1:D:117:SER:CB	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:ASP:HA	2:C:302:SO4:O2	2.16	0.46
1:D:151:TYR:HB3	1:D:152:PRO:HD2	1.98	0.46
1:B:25:GLU:HG3	1:B:26:ASN:N	2.32	0.45
1:B:166:GLU:CD	1:B:166:GLU:H	2.19	0.45
1:C:79:GLY:C	1:C:81:MET:H	2.18	0.45
1:A:33:ILE:HB	1:A:42:CYS:O	2.16	0.45
1:A:141:PHE:HD1	1:A:154:ASN:OD1	1.99	0.45
1:A:169:MET:HE1	1:D:171:TYR:CD2	2.51	0.45
1:A:70:GLN:O	1:A:79:GLY:HA2	2.16	0.45
1:B:168:CYS:O	1:B:170:GLN:N	2.51	0.45
1:A:36:LYS:HE3	1:A:65:VAL:HG23	1.98	0.45
1:B:153:LYS:HD2	1:B:153:LYS:HA	1.88	0.44
1:A:197:GLY:HA3	1:A:215:TRP:CZ2	2.52	0.44
1:D:197:GLY:HA3	1:D:215:TRP:CZ2	2.52	0.44
1:A:153:LYS:HA	1:A:153:LYS:HD2	1.73	0.44
1:A:140:GLY:CA	1:A:155:LEU:HD12	2.47	0.44
1:B:41:LYS:HD2	1:B:41:LYS:HA	1.78	0.44
1:A:57:HIS:ND1	1:A:102:ASP:OD2	2.51	0.44
1:A:116:ARG:HA	1:A:116:ARG:HD3	1.33	0.44
1:C:28:PRO:HB2	1:C:119:GLN:N	2.32	0.44
1:C:126:ARG:HH22	1:D:95:ARG:NE	2.16	0.44
1:B:172:TYR:HE2	1:D:172:TYR:HE2	1.65	0.44
1:A:169:MET:CE	1:D:171:TYR:CZ	2.98	0.44
1:C:36:LYS:HE3	1:C:65:VAL:HG23	2.00	0.44
1:C:51:TRP:CH2	1:C:107:LYS:HB2	2.53	0.44
1:A:97:ASP:C	1:A:97(B):LEU:H	2.20	0.44
1:B:25:GLU:HG3	1:B:26:ASN:H	1.83	0.43
1:D:25:GLU:N	1:D:157:MET:HG3	2.33	0.43
1:B:209:LEU:HG	1:B:231:VAL:HG21	2.00	0.43
1:A:165:HIS:NE2	1:A:183:ALA:O	2.40	0.43
1:A:169:MET:HE3	1:D:171:TYR:CZ	2.52	0.43
1:B:57:HIS:ND1	1:B:102:ASP:OD2	2.52	0.43
1:B:166:GLU:OE2	1:A:166:GLU:OE2	2.36	0.43
1:B:162:LEU:HD22	1:B:228:TYR:CE1	2.54	0.43
1:B:170:GLN:N	1:B:170(A):PRO:CD	2.81	0.43
1:C:126:ARG:HH21	1:C:126:ARG:HD2	1.54	0.43
1:B:163:VAL:HG11	1:B:180:MET:HE3	2.00	0.43
1:D:69:GLY:C	1:D:80:GLU:HG2	2.40	0.42
1:A:51:TRP:CH2	1:A:107:LYS:HB2	2.54	0.42
1:A:60(B):LEU:HD23	1:A:60(B):LEU:HA	1.89	0.42
1:B:28:PRO:HB2	1:B:119:GLN:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LEU:HD12	1:A:151:TYR:HE1	1.84	0.42
1:D:62:LYS:H	1:D:62:LYS:CD	2.03	0.42
1:D:196:GLY:HA2	1:D:214:SER:HA	2.01	0.42
1:D:212:ILE:HB	1:D:229:THR:HB	1.99	0.42
1:A:100:HIS:CD2	1:A:184:ALA:HB1	2.55	0.42
1:D:224:LYS:HA	1:D:225:PRO:HD3	1.80	0.42
1:B:138:ILE:O	1:B:157:MET:HA	2.20	0.42
1:A:25:GLU:N	1:A:27:GLN:HB2	2.35	0.42
1:A:138:ILE:O	1:A:157:MET:HA	2.20	0.42
1:C:197:GLY:HA3	1:C:215:TRP:CZ2	2.55	0.42
1:D:97(B):LEU:HA	1:D:97(B):LEU:HD12	1.84	0.42
1:B:36:LYS:HE3	1:B:65:VAL:CG2	2.50	0.42
1:B:168:CYS:O	1:B:169:MET:CG	2.68	0.42
1:B:224:LYS:HA	1:B:225:PRO:HD3	1.92	0.42
1:B:27:GLN:HB3	1:B:28:PRO:HD2	2.01	0.42
1:C:36:LYS:NZ	1:C:84:GLU:OE1	2.44	0.42
1:C:68:LEU:O	1:C:80:GLU:N	2.52	0.42
1:D:163:VAL:HG11	1:D:180:MET:HE3	2.01	0.41
1:A:61:LYS:HA	1:A:61:LYS:HD3	1.84	0.41
1:B:28:PRO:HB2	1:B:119:GLN:H	1.84	0.41
1:C:68:LEU:HB3	1:C:118:ILE:HD12	2.01	0.41
1:C:126:ARG:NH1	1:D:95:ARG:HD3	2.30	0.41
1:B:164:SER:HB2	1:B:166:GLU:OE2	2.19	0.41
1:D:69:GLY:CA	1:D:80:GLU:OE1	2.68	0.41
1:A:206:ARG:HE	1:A:206:ARG:HB2	1.57	0.41
1:D:70:GLN:H	1:D:80:GLU:CG	2.28	0.41
1:C:196:GLY:HA2	1:C:214:SER:HA	2.03	0.41
1:D:162:LEU:HD22	1:D:228:TYR:CE1	2.55	0.41
1:C:162:LEU:HD22	1:C:228:TYR:CE1	2.55	0.41
1:B:168:CYS:C	1:B:169:MET:CG	2.88	0.40
1:A:140:GLY:C	1:A:155:LEU:HD12	2.42	0.40
1:B:33:ILE:HB	1:B:42:CYS:O	2.21	0.40
1:B:138:ILE:HG22	1:B:199:LEU:HG	2.03	0.40
1:A:170:GLN:H	1:A:170(A):PRO:HD3	1.86	0.40
1:A:209:LEU:HG	1:A:231:VAL:HG21	2.03	0.40
1:A:196:GLY:HA2	1:A:214:SER:HA	2.03	0.40
1:C:36:LYS:HE3	1:C:65:VAL:CG2	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	218/247 (88%)	204 (94%)	11 (5%)	3 (1%)	11	40
1	B	218/247 (88%)	201 (92%)	14 (6%)	3 (1%)	11	40
1	C	218/247 (88%)	197 (90%)	16 (7%)	5 (2%)	6	27
1	D	218/247 (88%)	200 (92%)	16 (7%)	2 (1%)	17	52
All	All	872/988 (88%)	802 (92%)	57 (6%)	13 (2%)	10	39

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170	GLN
1	B	169	MET
1	A	152	PRO
1	A	154	ASN
1	D	152	PRO
1	C	37(D)	SER
1	D	37(D)	SER
1	B	153	LYS
1	C	36	LYS
1	B	170	GLN
1	C	37(C)	GLY
1	C	37(E)	PRO
1	C	43	GLY

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	191/212 (90%)	185 (97%)	6 (3%)	40	73
1	B	191/212 (90%)	186 (97%)	5 (3%)	46	76
1	C	191/212 (90%)	183 (96%)	8 (4%)	30	64
1	D	191/212 (90%)	186 (97%)	5 (3%)	46	76
All	All	764/848 (90%)	740 (97%)	24 (3%)	40	73

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	35	GLN
1	B	37(A)	LYS
1	B	37(D)	SER
1	B	109	ARG
1	B	222	GLU
1	A	37(D)	SER
1	A	151	TYR
1	A	153	LYS
1	A	169	MET
1	A	182	CYS
1	A	187	LYS
1	C	35	GLN
1	C	37	ASN
1	C	37(D)	SER
1	C	39	SER
1	C	40	PHE
1	C	42	CYS
1	C	156	LYS
1	C	187	LYS
1	D	37(A)	LYS
1	D	37(D)	SER
1	D	39	SER
1	D	62	LYS
1	D	95	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	35	GLN
1	C	167	GLN
1	D	37	ASN
1	D	170	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	C	302	-	4,4,4	0.09	0	6,6,6	0.24	0
2	SO4	D	301	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	A	301	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	A	302	-	4,4,4	0.14	0	6,6,6	0.05	0
2	SO4	C	301	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	D	302	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	B	301	-	4,4,4	0.14	0	6,6,6	0.06	0
2	SO4	B	302	-	4,4,4	0.14	0	6,6,6	0.06	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	302	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, 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	224/247 (90%)	0.37	6 (2%)	54	26	46, 71, 125, 162	0
1	B	224/247 (90%)	0.36	7 (3%)	49	22	42, 70, 121, 167	0
1	C	224/247 (90%)	0.37	8 (3%)	42	18	41, 70, 124, 160	0
1	D	224/247 (90%)	0.37	4 (1%)	68	40	42, 70, 129, 157	0
All	All	896/988 (90%)	0.37	25 (2%)	53	24	41, 70, 126, 167	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	221	ALA	5.6
1	D	78	PRO	5.0
1	B	119	GLN	3.6
1	C	40	PHE	3.5
1	B	165	HIS	3.0
1	D	119	GLN	2.9
1	C	177	ASN	2.7
1	B	40	PHE	2.7
1	D	118	ILE	2.5
1	B	152	PRO	2.5
1	C	37(C)	GLY	2.4
1	A	172	TYR	2.3
1	B	112	ALA	2.3
1	A	153	LYS	2.2
1	C	167	GLN	2.2
1	C	108	ILE	2.2
1	D	191	CYS	2.1
1	C	103	ILE	2.1
1	A	112	ALA	2.1
1	B	78	PRO	2.1
1	C	126	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	170	GLN	2.1
1	A	68	LEU	2.1
1	A	33	ILE	2.0
1	A	187	LYS	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	C	302	5/5	0.28	0.43	179,182,183,183	0
2	SO4	D	302	5/5	0.75	0.31	162,165,166,170	0
2	SO4	B	302	5/5	0.77	0.31	150,152,155,155	0
2	SO4	A	302	5/5	0.79	0.36	163,164,167,167	0
2	SO4	C	301	5/5	0.80	0.24	126,134,140,140	0
2	SO4	B	301	5/5	0.83	0.29	141,146,147,149	0
3	NI	C	303	1/1	0.83	0.09	114,114,114,114	0
3	NI	B	303	1/1	0.84	0.12	120,120,120,120	0
2	SO4	A	301	5/5	0.84	0.19	124,125,128,133	0
3	NI	C	304	1/1	0.85	0.15	130,130,130,130	0
2	SO4	D	301	5/5	0.87	0.15	143,143,146,146	0
3	NI	A	303	1/1	0.90	0.15	120,120,120,120	0

6.5 Other polymers (i)

There are no such residues in this entry.