Full wwPDB X-ray Structure Validation Report ⓘ

Dec 18, 2023 – 05:35 am GMT

PDB ID	:	3ZGB
Title	:	Greater efficiency of photosynthetic carbon fixation due to single amino acid substitution
Authors	:	Paulus, J.K.; Schlieper, D.; Groth, G.
Deposited on	:	2012-12-17
Resolution	:	2.71 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:

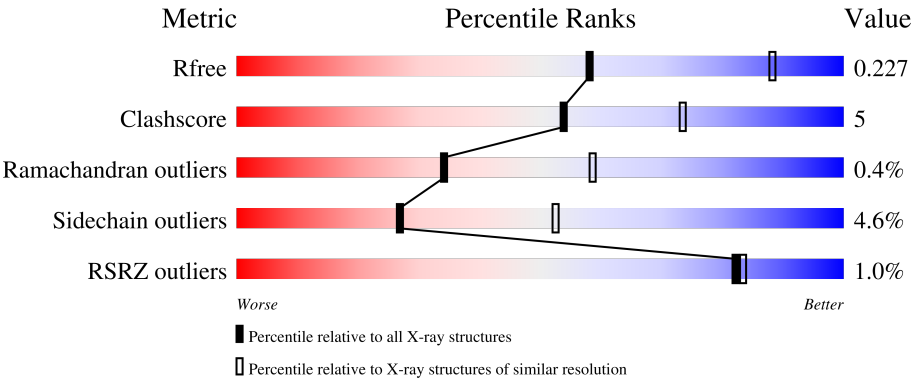
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

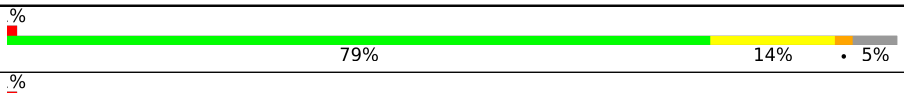
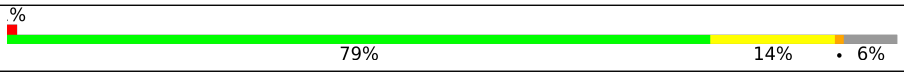
The reported resolution of this entry is 2.71 Å.

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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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	972	
1	B	972	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 14852 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 PHOSPHOENOLPYRUVATE CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	920	Total	C	N	O	S	0	0	0
			7396	4691	1289	1382	34			
1	B	915	Total	C	N	O	S	0	0	0
			7354	4663	1282	1375	34			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	expression tag	UNP Q01647
A	-4	GLY	-	expression tag	UNP Q01647
A	-3	HIS	-	expression tag	UNP Q01647
A	-2	HIS	-	expression tag	UNP Q01647
A	-1	HIS	-	expression tag	UNP Q01647
A	0	HIS	-	expression tag	UNP Q01647
A	1	HIS	-	expression tag	UNP Q01647
A	2	HIS	-	expression tag	UNP Q01647
A	3	HIS	-	expression tag	UNP Q01647
A	4	HIS	-	expression tag	UNP Q01647
A	5	HIS	-	expression tag	UNP Q01647
A	?	-	LYS	SEE REMARK 999	UNP Q01647
A	291	ASN	HIS	SEE REMARK 999	UNP Q01647
B	-5	MET	-	expression tag	UNP Q01647
B	-4	GLY	-	expression tag	UNP Q01647
B	-3	HIS	-	expression tag	UNP Q01647
B	-2	HIS	-	expression tag	UNP Q01647
B	-1	HIS	-	expression tag	UNP Q01647
B	0	HIS	-	expression tag	UNP Q01647
B	1	HIS	-	expression tag	UNP Q01647
B	2	HIS	-	expression tag	UNP Q01647
B	3	HIS	-	expression tag	UNP Q01647
B	4	HIS	-	expression tag	UNP Q01647
B	5	HIS	-	expression tag	UNP Q01647
B	?	-	LYS	SEE REMARK 999	UNP Q01647

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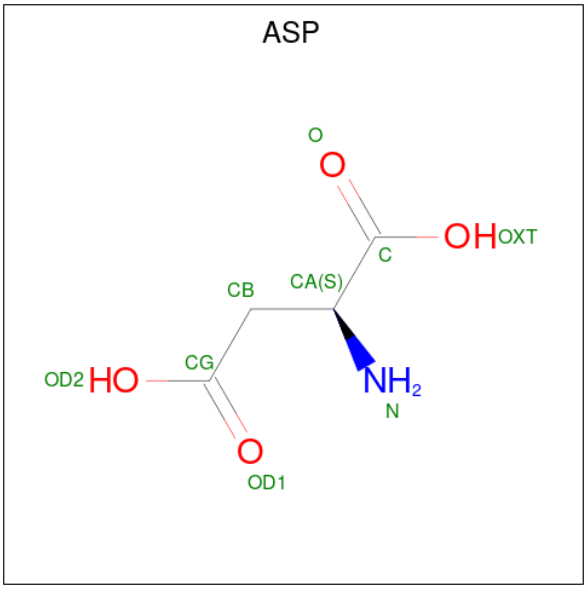
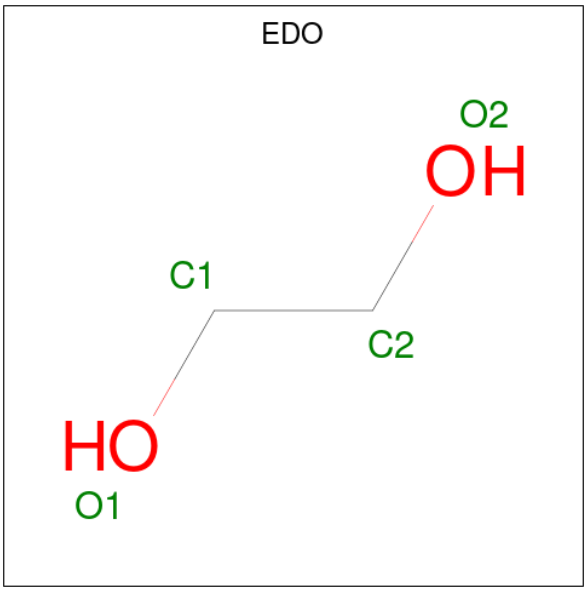
Chain	Residue	Modelled	Actual	Comment	Reference
B	291	ASN	HIS	SEE REMARK 999	UNP Q01647

- Molecule 2 is ASPARTIC ACID (three-letter code: ASP) (formula: $C_4H_7NO_4$).



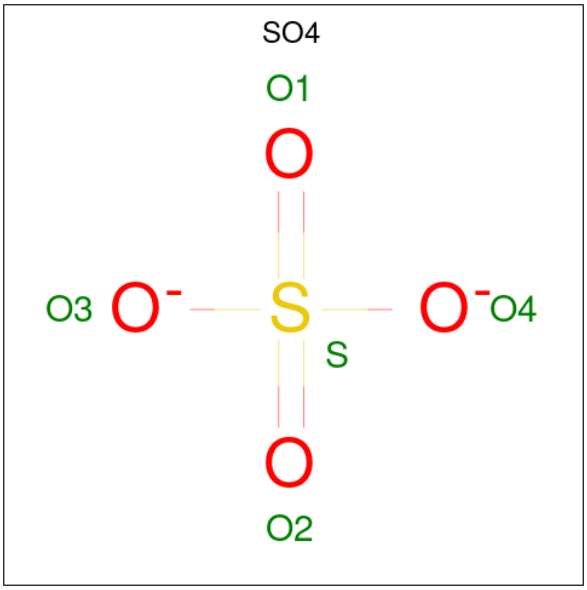
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			9	4	1	4		
2	B	1	Total	C	N	O	0	0
			9	4	1	4		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

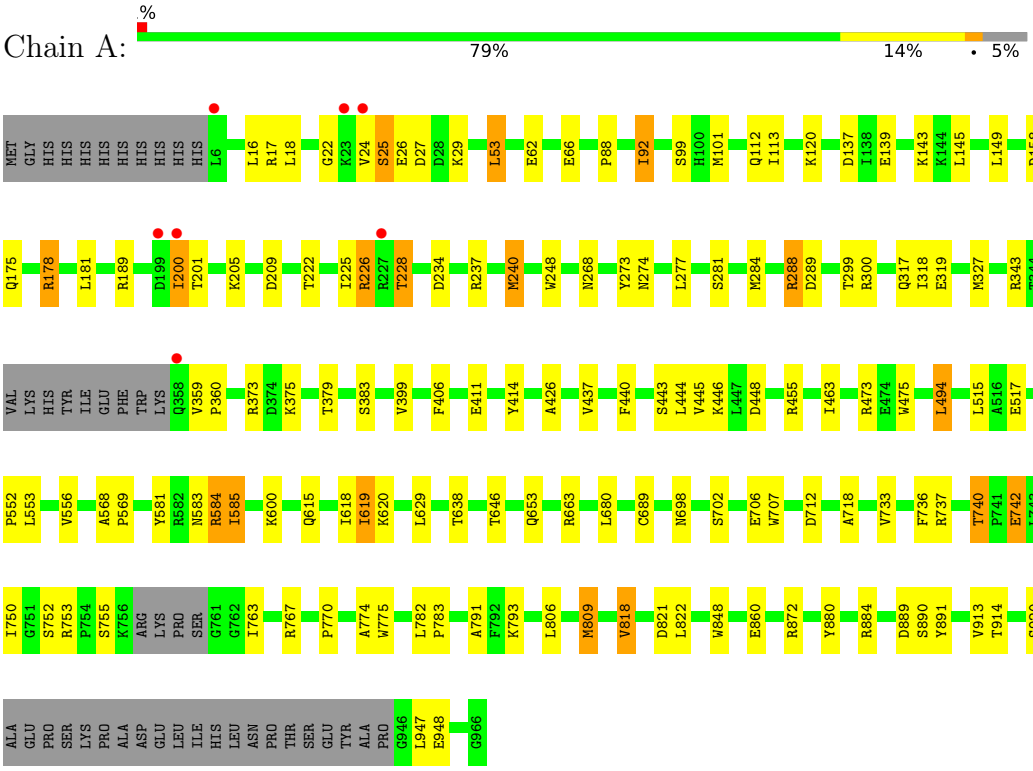
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	35	Total O 35 35	0	0
5	B	21	Total O 21 21	0	0

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.

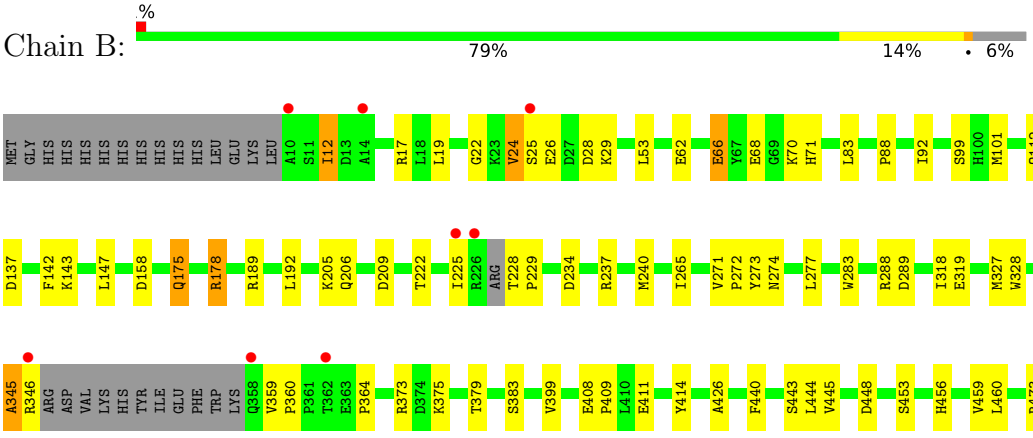
• Molecule 1: PHOSPHOENOLPYRUVATE CARBOXYLASE

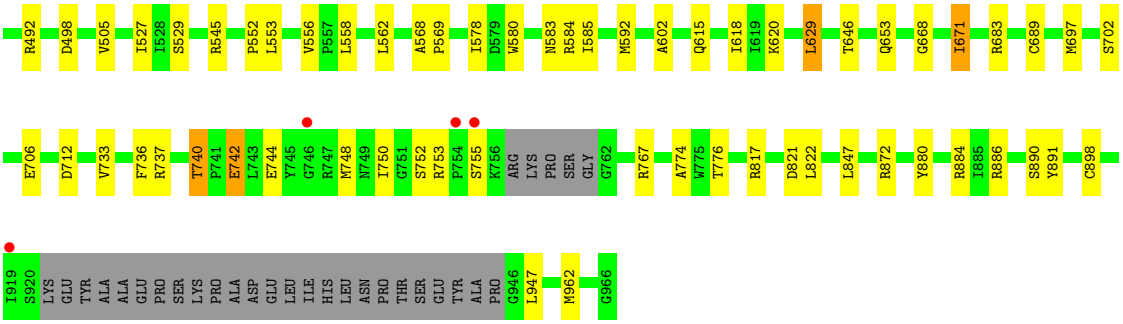
Chain A:



• Molecule 1: PHOSPHOENOLPYRUVATE CARBOXYLASE

Chain B:




R492 D498 V505 I527 I528 S529 R545 P552 L553 V556 P557 L558 L562 A568 P569 I578 D579 W580 N583 R584 I585 M592 A602 Q615 I618 I619 K620 L629 T646 Q653 G668 I671 R683 C689 M697 S702
E706 D712 V733 F736 R737 T740 P741 E742 L743 E744 Y745 G746 R747 M748 N749 I750 G751 S752 R753 P754 S755 K756 ARG LYS PRO SER GLY G762 R767 A774 W775 T776 R817 D821 L822 L847 R872 Y880 R884 I885 R886 S890 Y891 C898
I919 S920 LYS GLU TYR ALA ALA GLU PRO SER LYS PRO ALA ASP GLU LEU ILE HIS LEU ASN PRO THR SER GLU TYR ALA PRO G946 L947 M962 G966

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	165.55Å 121.70Å 132.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.72 – 2.71 70.13 – 2.71	Depositor EDS
% Data completeness (in resolution range)	100.0 (78.72-2.71) 100.0 (70.13-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	10.98 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.188 , 0.230 0.188 , 0.227	Depositor DCC
R_{free} test set	1486 reflections (2.03%)	wwPDB-VP
Wilson B-factor (Å^2)	45.2	Xtriage
Anisotropy	0.657	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 32.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14852	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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: SO4, EDO

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	0.90	5/7549 (0.1%)	0.95	22/10205 (0.2%)
1	B	0.80	2/7506 (0.0%)	0.89	16/10148 (0.2%)
All	All	0.85	7/15055 (0.0%)	0.92	38/20353 (0.2%)

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	B	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	283	TRP	CD2-CE2	5.54	1.48	1.41
1	A	475	TRP	NE1-CE2	-5.50	1.30	1.37
1	B	328	TRP	CD2-CE2	5.49	1.48	1.41
1	A	848	TRP	CD2-CE2	5.31	1.47	1.41
1	A	775	TRP	CD2-CE2	5.21	1.47	1.41
1	A	707	TRP	CD2-CE2	5.15	1.47	1.41
1	A	517	GLU	CD-OE1	5.10	1.31	1.25

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	455	ARG	NE-CZ-NH2	-10.03	115.28	120.30
1	A	455	ARG	NE-CZ-NH1	9.96	125.28	120.30
1	A	821	ASP	CB-CG-OD2	-8.32	110.81	118.30
1	A	889	ASP	CB-CG-OD2	-8.29	110.84	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	821	ASP	CB-CG-OD1	7.74	125.27	118.30
1	A	448	ASP	CB-CG-OD1	7.46	125.01	118.30
1	B	448	ASP	CB-CG-OD1	7.27	124.84	118.30
1	B	821	ASP	CB-CG-OD1	7.04	124.63	118.30
1	B	817	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	A	494	LEU	CB-CG-CD1	-6.86	99.34	111.00
1	B	821	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	A	137	ASP	CB-CG-OD1	6.64	124.27	118.30
1	B	697	MET	CG-SD-CE	-6.62	89.62	100.20
1	A	443	SER	C-N-CA	-6.56	105.31	121.70
1	B	288	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	A	189	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	A	288	ARG	NE-CZ-NH2	-6.21	117.20	120.30
1	A	712	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	663	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	889	ASP	CB-CG-OD1	5.83	123.55	118.30
1	B	443	SER	C-N-CA	-5.82	107.14	121.70
1	A	446	LYS	CD-CE-NZ	-5.61	98.80	111.70
1	A	473	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	B	492	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	689	CYS	CA-CB-SG	-5.42	104.24	114.00
1	B	683	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	B	712	ASP	CB-CG-OD1	5.36	123.12	118.30
1	A	584	ARG	CG-CD-NE	-5.35	100.56	111.80
1	A	300	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	92	ILE	CG1-CB-CG2	-5.31	99.71	111.40
1	B	189	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	343	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	663	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	B	137	ASP	CB-CG-OD1	5.26	123.04	118.30
1	B	689	CYS	CA-CB-SG	-5.17	104.69	114.00
1	B	473	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	B	192	LEU	CB-CG-CD2	-5.07	102.38	111.00
1	A	240	MET	CG-SD-CE	-5.01	92.18	100.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	229	PRO	Peptide

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	7396	0	7381	83	0
1	B	7354	0	7328	75	0
2	A	9	0	3	0	0
2	B	9	0	3	0	0
3	A	4	0	6	0	0
3	B	4	0	6	1	0
4	A	10	0	0	1	0
4	B	10	0	0	1	0
5	A	35	0	0	0	0
5	B	21	0	0	0	0
All	All	14852	0	14727	155	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 5.

All (155) 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:806:LEU:HA	1:A:809:MET:HE2	1.39	1.04
1:A:806:LEU:HD23	1:A:809:MET:HE1	1.49	0.94
1:B:273:TYR:OH	1:B:411:GLU:OE2	1.90	0.90
1:A:273:TYR:OH	1:A:411:GLU:OE2	1.92	0.86
1:B:488:LEU:O	1:B:545:ARG:NH2	2.11	0.83
1:B:379:THR:HA	1:B:399:VAL:HG22	1.64	0.78
1:A:615:GLN:HE22	1:A:653:GLN:HE22	1.31	0.77
1:B:615:GLN:HE22	1:B:653:GLN:HE22	1.30	0.77
1:A:806:LEU:HD23	1:A:809:MET:CE	2.14	0.76
1:B:318:ILE:CG2	1:B:373:ARG:HG3	2.16	0.76
1:A:178:ARG:NH1	4:A:1969:SO4:O2	2.21	0.74
1:A:200:ILE:HG22	1:A:201:THR:H	1.53	0.74
1:B:615:GLN:HE22	1:B:653:GLN:NE2	1.85	0.73
1:A:318:ILE:CG2	1:A:373:ARG:HG3	2.18	0.73
1:A:240:MET:HE2	1:A:284:MET:HE1	1.71	0.72
1:A:615:GLN:HE22	1:A:653:GLN:NE2	1.90	0.69
1:A:120:LYS:NZ	1:B:24:VAL:HG23	2.08	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:ILE:HG22	1:A:629:LEU:HD22	1.74	0.68
1:B:618:ILE:HG22	1:B:629:LEU:HD22	1.76	0.68
1:A:240:MET:CE	1:A:284:MET:HE1	2.24	0.67
1:A:806:LEU:HA	1:A:809:MET:CE	2.20	0.67
1:A:240:MET:CE	1:A:284:MET:CE	2.72	0.67
1:A:29:LYS:H	1:A:112:GLN:HE22	1.43	0.66
1:B:289:ASP:O	1:B:767:ARG:NH1	2.27	0.66
1:A:359:VAL:HG13	1:A:360:PRO:HD2	1.77	0.66
1:B:222:THR:HG22	1:B:222:THR:O	1.96	0.65
1:A:240:MET:HE3	1:A:284:MET:HE3	1.79	0.65
1:A:289:ASP:O	1:A:767:ARG:NH1	2.28	0.65
1:B:240:MET:HE3	1:B:445:VAL:HG21	1.79	0.64
1:A:120:LYS:HZ1	1:B:24:VAL:HG23	1.65	0.62
1:B:62:GLU:O	1:B:66:GLU:HG2	2.00	0.62
1:B:562:LEU:HD13	1:B:602:ALA:CB	2.30	0.61
1:B:736:PHE:O	1:B:740:THR:HB	2.01	0.61
1:B:379:THR:CA	1:B:399:VAL:HG22	2.32	0.60
1:B:29:LYS:H	1:B:112:GLN:HE22	1.47	0.59
1:A:379:THR:HA	1:A:399:VAL:HG22	1.83	0.59
1:B:19:LEU:HD11	1:B:68:GLU:HB2	1.83	0.59
1:B:568:ALA:HB3	1:B:569:PRO:HD3	1.84	0.59
1:A:240:MET:HE3	1:A:284:MET:CE	2.33	0.59
1:A:226:ARG:NH1	1:A:228:THR:OG1	2.36	0.59
1:B:273:TYR:CE1	1:B:274:ASN:HB3	2.39	0.58
1:A:145:LEU:HD23	1:A:149:LEU:HD13	1.86	0.58
1:A:736:PHE:O	1:A:740:THR:HB	2.03	0.58
1:A:248:TRP:HE1	1:A:317:GLN:HE21	1.52	0.57
1:A:740:THR:HG22	1:A:742:GLU:H	1.69	0.56
1:B:178:ARG:NH1	4:B:1969:SO4:O1	2.37	0.56
1:A:414:TYR:CE1	1:A:426:ALA:HB1	2.41	0.56
1:A:414:TYR:CD1	1:A:426:ALA:HB1	2.41	0.56
1:A:618:ILE:HG22	1:A:629:LEU:CD2	2.35	0.55
1:A:139:GLU:OE2	1:A:143:LYS:NZ	2.40	0.55
1:B:552:PRO:HB2	1:B:584:ARG:NH2	2.22	0.54
1:A:638:THR:HG21	1:A:818:VAL:HG13	1.89	0.54
1:B:12:ILE:HD12	1:B:12:ILE:H	1.72	0.54
1:A:748:MET:HE1	1:A:948:GLU:HB3	1.90	0.54
1:A:24:VAL:HG12	1:B:120:LYS:NZ	2.23	0.53
1:B:440:PHE:HB3	1:B:444:LEU:HD23	1.89	0.53
1:A:318:ILE:HG21	1:A:373:ARG:HG3	1.91	0.53
1:A:359:VAL:CG1	1:A:360:PRO:HD2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:VAL:HG13	1:B:360:PRO:HD2	1.90	0.53
1:B:736:PHE:CE2	1:B:742:GLU:HG2	2.43	0.52
1:B:822:LEU:HD11	3:B:1968:EDO:H22	1.91	0.52
1:A:25:SER:HB2	1:A:27:ASP:OD1	2.09	0.52
1:A:736:PHE:CE2	1:A:742:GLU:HG2	2.44	0.52
1:B:880:TYR:O	1:B:884:ARG:HG3	2.09	0.52
1:B:318:ILE:HG21	1:B:373:ARG:HG3	1.89	0.52
1:A:880:TYR:O	1:A:884:ARG:HG3	2.10	0.52
1:A:319:GLU:OE2	1:A:373:ARG:HD2	2.10	0.51
1:B:319:GLU:OE2	1:B:373:ARG:HD2	2.10	0.51
1:A:463:ILE:HG21	1:A:494:LEU:HD13	1.92	0.51
1:B:277:LEU:HD12	1:B:277:LEU:N	2.25	0.51
1:A:619:ILE:HD12	1:A:629:LEU:HD22	1.93	0.51
1:A:552:PRO:HB2	1:A:584:ARG:NH2	2.25	0.51
1:B:488:LEU:HD22	1:B:580:TRP:CZ2	2.45	0.51
1:A:200:ILE:HB	1:A:205:LYS:HE3	1.91	0.51
1:B:488:LEU:HD22	1:B:580:TRP:CH2	2.46	0.50
1:A:740:THR:CG2	1:A:742:GLU:HB3	2.42	0.50
1:A:359:VAL:HG12	1:A:360:PRO:N	2.27	0.50
1:A:581:TYR:CZ	1:A:585:ILE:HD13	2.47	0.50
1:A:568:ALA:HB3	1:A:569:PRO:HD3	1.95	0.49
1:A:733:VAL:O	1:A:737:ARG:HG3	2.13	0.49
1:A:273:TYR:CE1	1:A:274:ASN:HB3	2.47	0.49
1:A:748:MET:CE	1:A:948:GLU:HB3	2.42	0.48
1:B:733:VAL:O	1:B:737:ARG:HG3	2.13	0.48
1:B:414:TYR:CD1	1:B:426:ALA:HB1	2.49	0.48
1:A:53:LEU:HD13	1:A:920:SER:HB3	1.96	0.48
1:B:234:ASP:OD1	1:B:237:ARG:NH2	2.47	0.48
1:B:618:ILE:HG22	1:B:629:LEU:CD2	2.41	0.48
1:A:379:THR:CA	1:A:399:VAL:HG22	2.44	0.47
1:B:143:LYS:O	1:B:147:LEU:HD23	2.14	0.47
1:B:740:THR:CG2	1:B:774:ALA:HB1	2.44	0.47
1:B:359:VAL:CG1	1:B:360:PRO:HD2	2.43	0.47
1:B:558:LEU:HD13	1:B:592:MET:HG2	1.95	0.47
1:A:113:ILE:HG22	1:A:680:LEU:HD21	1.96	0.47
1:B:142:PHE:HB3	1:B:265:ILE:HD13	1.96	0.47
1:A:288:ARG:NH2	1:A:299:THR:OG1	2.33	0.47
1:B:88:PRO:O	1:B:92:ILE:HD13	2.14	0.47
1:B:28:ASP:HA	1:B:112:GLN:HE22	1.80	0.47
1:A:234:ASP:OD1	1:A:237:ARG:NH2	2.48	0.46
1:A:222:THR:HG22	1:A:222:THR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:LEU:HD13	1:B:602:ALA:HB3	1.96	0.46
1:A:740:THR:CG2	1:A:742:GLU:H	2.28	0.46
1:A:527:ILE:HD13	1:A:556:VAL:HB	1.97	0.46
1:B:175:GLN:OE1	1:B:750:ILE:HG23	2.16	0.46
1:B:343:ARG:O	1:B:345:ALA:N	2.49	0.46
1:B:344:THR:O	1:B:346:ARG:N	2.49	0.46
1:B:740:THR:CG2	1:B:742:GLU:HB3	2.46	0.46
1:A:744:GLU:O	1:A:748:MET:HG3	2.16	0.45
1:B:744:GLU:O	1:B:748:MET:HG3	2.17	0.45
1:B:460:LEU:HD23	1:B:460:LEU:HA	1.70	0.45
1:A:581:TYR:CZ	1:A:585:ILE:CD1	2.99	0.45
1:B:740:THR:HG22	1:B:742:GLU:H	1.81	0.45
1:B:553:LEU:HD12	1:B:553:LEU:N	2.31	0.45
1:A:62:GLU:O	1:A:66:GLU:HG3	2.17	0.45
1:B:527:ILE:HD13	1:B:556:VAL:HB	1.99	0.45
1:A:445:VAL:HG23	1:A:445:VAL:O	2.17	0.44
1:A:101:MET:HE3	1:A:891:TYR:CE1	2.52	0.44
1:B:847:LEU:HD23	1:B:847:LEU:HA	1.87	0.44
1:A:318:ILE:HG23	1:A:373:ARG:HG3	1.99	0.43
1:A:913:VAL:HG12	1:A:914:THR:N	2.32	0.43
1:A:406:PHE:CE2	1:A:437:VAL:HG22	2.54	0.43
1:A:740:THR:CG2	1:A:774:ALA:HB1	2.49	0.43
1:A:101:MET:HE3	1:A:891:TYR:HE1	1.83	0.43
1:B:459:VAL:HG22	1:B:505:VAL:HG13	1.99	0.43
1:B:83:LEU:HD13	1:B:898:CYS:HB2	2.00	0.43
1:A:822:LEU:C	1:A:822:LEU:HD23	2.39	0.43
1:A:174:THR:HA	1:A:750:ILE:HG22	2.00	0.43
1:A:440:PHE:HB3	1:A:444:LEU:HD23	2.01	0.42
1:A:782:LEU:HB3	1:A:783:PRO:HD3	2.01	0.42
1:B:101:MET:HE3	1:B:891:TYR:CE1	2.54	0.42
1:B:668:GLY:O	1:B:671:ILE:HG13	2.18	0.42
1:A:767:ARG:O	1:A:770:PRO:HD2	2.19	0.42
1:B:70:LYS:O	1:B:71:HIS:HB2	2.19	0.42
1:B:553:LEU:N	1:B:553:LEU:CD1	2.82	0.42
1:A:166:ASP:OD1	1:A:281:SER:OG	2.36	0.42
1:A:553:LEU:N	1:A:553:LEU:CD1	2.83	0.42
1:B:359:VAL:HG12	1:B:360:PRO:N	2.35	0.42
1:B:488:LEU:C	1:B:545:ARG:HH22	2.19	0.42
1:B:776:THR:HG22	1:B:962:MET:HG3	2.02	0.42
1:B:334:LEU:CD2	1:B:364:PRO:HB2	2.50	0.42
1:A:88:PRO:O	1:A:92:ILE:HD13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:793:LYS:NZ	1:A:860:GLU:OE1	2.52	0.41
1:A:600:LYS:NZ	1:A:763:ILE:O	2.52	0.41
1:B:485:LEU:HD21	1:B:578:ILE:HG21	2.02	0.41
1:B:453:SER:HA	1:B:456:HIS:HD1	1.85	0.41
1:B:668:GLY:HA2	1:B:671:ILE:CG1	2.50	0.41
1:A:515:LEU:HD13	1:A:553:LEU:HD22	2.03	0.41
1:A:718:ALA:HB2	1:A:791:ALA:HB2	2.03	0.41
1:A:181:LEU:HD12	1:A:181:LEU:HA	1.82	0.41
1:B:562:LEU:HD13	1:B:602:ALA:HB2	2.03	0.41
1:B:205:LYS:O	1:B:206:GLN:C	2.60	0.41
1:B:271:VAL:O	1:B:272:PRO:C	2.57	0.41
1:B:318:ILE:HG23	1:B:373:ARG:HG3	2.01	0.40
1:A:277:LEU:HD12	1:A:277:LEU:N	2.36	0.40
1:B:143:LYS:O	1:B:147:LEU:CD2	2.70	0.40
1:B:408:GLU:HB3	1:B:409:PRO:CD	2.52	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	912/972 (94%)	879 (96%)	30 (3%)	3 (0%)	41	65
1	B	905/972 (93%)	873 (96%)	27 (3%)	5 (1%)	25	48
All	All	1817/1944 (94%)	1752 (96%)	57 (3%)	8 (0%)	34	58

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	752	SER
1	B	752	SER
1	A	22	GLY

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Mol	Chain	Res	Type
1	B	22	GLY
1	B	498	ASP
1	B	345	ALA
1	A	175	GLN
1	B	175	GLN

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	802/848 (95%)	765 (95%)	37 (5%)	27	52
1	B	797/848 (94%)	761 (96%)	36 (4%)	27	53
All	All	1599/1696 (94%)	1526 (95%)	73 (5%)	27	52

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	17	ARG
1	A	18	LEU
1	A	25	SER
1	A	26	GLU
1	A	53	LEU
1	A	99	SER
1	A	158	ASP
1	A	178	ARG
1	A	200	ILE
1	A	209	ASP
1	A	225	ILE
1	A	226	ARG
1	A	228	THR
1	A	268	ASN
1	A	327	MET
1	A	343	ARG
1	A	375	LYS

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Mol	Chain	Res	Type
1	A	383	SER
1	A	529	SER
1	A	583	ASN
1	A	585	ILE
1	A	619	ILE
1	A	620	LYS
1	A	646	THR
1	A	698	ASN
1	A	702	SER
1	A	706	GLU
1	A	740	THR
1	A	742	GLU
1	A	753	ARG
1	A	755	SER
1	A	809	MET
1	A	818	VAL
1	A	872	ARG
1	A	890	SER
1	A	947	LEU
1	B	12	ILE
1	B	17	ARG
1	B	24	VAL
1	B	25	SER
1	B	26	GLU
1	B	53	LEU
1	B	66	GLU
1	B	99	SER
1	B	121	LEU
1	B	158	ASP
1	B	178	ARG
1	B	209	ASP
1	B	225	ILE
1	B	228	THR
1	B	327	MET
1	B	343	ARG
1	B	344	THR
1	B	375	LYS
1	B	383	SER
1	B	529	SER
1	B	583	ASN
1	B	585	ILE
1	B	620	LYS

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Mol	Chain	Res	Type
1	B	629	LEU
1	B	646	THR
1	B	671	ILE
1	B	702	SER
1	B	706	GLU
1	B	740	THR
1	B	742	GLU
1	B	753	ARG
1	B	755	SER
1	B	872	ARG
1	B	886	ARG
1	B	890	SER
1	B	947	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	A	194	GLN
1	A	317	GLN
1	A	358	GLN
1	A	610	GLN
1	A	653	GLN
1	A	673	GLN
1	A	698	ASN
1	A	781	HIS
1	A	963	GLN
1	B	112	GLN
1	B	150	ASN
1	B	389	HIS
1	B	653	GLN
1	B	673	GLN
1	B	781	HIS
1	B	963	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ASP	A	1967	-	6,8,8	1.46	1 (16%)	8,10,10	1.25	0
4	SO4	B	1970	-	4,4,4	0.55	0	6,6,6	0.67	0
4	SO4	A	1970	-	4,4,4	0.46	0	6,6,6	0.27	0
2	ASP	B	1967	-	6,8,8	1.37	0	8,10,10	1.20	1 (12%)
3	EDO	A	1968	-	3,3,3	0.89	0	2,2,2	0.42	0
3	EDO	B	1968	-	3,3,3	0.65	0	2,2,2	0.20	0
4	SO4	A	1969	-	4,4,4	0.32	0	6,6,6	1.37	1 (16%)
4	SO4	B	1969	-	4,4,4	0.48	0	6,6,6	0.71	0

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
3	EDO	B	1968	-	-	1/1/1/1	-
2	ASP	A	1967	-	-	0/8/8/8	-
3	EDO	A	1968	-	-	1/1/1/1	-
2	ASP	B	1967	-	-	0/8/8/8	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1967	ASP	OXT-C	-2.14	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1969	SO4	O4-S-O3	2.47	119.59	109.06
2	B	1967	ASP	OD1-CG-CB	-2.17	115.86	122.80

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1968	EDO	O1-C1-C2-O2
3	B	1968	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1968	EDO	1	0
4	A	1969	SO4	1	0
4	B	1969	SO4	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	920/972 (94%)	-0.20	7 (0%)	86	87	23, 39, 78, 116	0
1	B	915/972 (94%)	-0.08	12 (1%)	77	78	29, 46, 88, 135	0
All	All	1835/1944 (94%)	-0.14	19 (1%)	82	83	23, 43, 83, 135	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	346	ARG	4.8
1	B	755	SER	4.4
1	B	754	PRO	4.0
1	B	919	ILE	3.5
1	A	358	GLN	3.3
1	A	199	ASP	3.1
1	A	6	LEU	3.1
1	B	746	GLY	2.9
1	B	25	SER	2.8
1	B	226	ARG	2.8
1	A	227	ARG	2.8
1	B	362	THR	2.7
1	B	358	GLN	2.5
1	B	10	ALA	2.4
1	A	23	LYS	2.4
1	B	225	ILE	2.4
1	A	24	VAL	2.3
1	A	200	ILE	2.2
1	B	14	ALA	2.2

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

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

6.3 Carbohydrates (i)

There are no 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
4	SO4	B	1970	5/5	0.91	0.21	60,72,86,87	0
3	EDO	A	1968	4/4	0.93	0.20	27,29,32,37	0
4	SO4	B	1969	5/5	0.94	0.16	55,64,69,76	0
2	ASP	A	1967	9/9	0.95	0.16	37,39,46,47	0
3	EDO	B	1968	4/4	0.95	0.24	31,36,37,39	0
4	SO4	A	1969	5/5	0.96	0.14	40,52,55,59	0
4	SO4	A	1970	5/5	0.96	0.14	63,64,80,87	0
2	ASP	B	1967	9/9	0.97	0.16	34,41,46,47	0

6.5 Other polymers (i)

There are no such residues in this entry.