Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:00 PM GMT

PDB ID : 1RM5

Title : Crystal structure of mutant S188A of photosynthetic glyceraldehyde-3-phosphate dehydrogenase A4 isoform, complexed with NADP

Authors : Sparla, F.; Fermani, S.; Falini, G.; Ripamonti, A.; Sabatino, P.; Pupillo, P.; Trost, P.

Deposited on : 2003-11-27

Resolution : 2.10 Å(reported)

The following versions of software and data (see references (i)) 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 ⓘ

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

The reported resolution of this entry is 2.10 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	Percentile Ranks	Value
Rfree		0.257
Clashscore		7
Ramachandran outliers		0.3%
Sidechain outliers		2.6%
RSRZ outliers		4.5%

Worse ← → *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
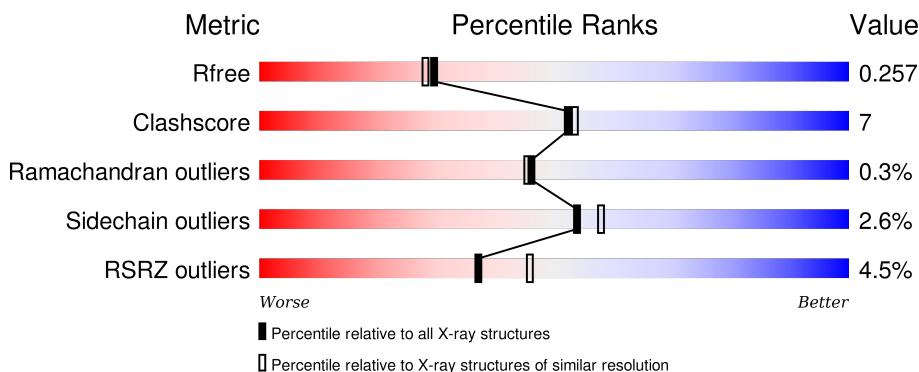
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	337	3% / 85% / 13% / •
1	B	337	10% / 88% / 10% / •
1	O	337	% / 88% / 9% / •
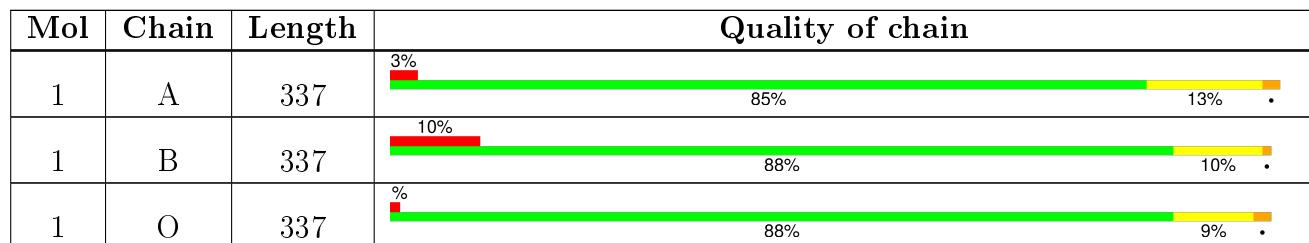
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	1339	-	-	-	X
2	SO4	B	2339	-	-	-	X
2	SO4	O	902	-	-	-	X
3	NDP	A	1335	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8363 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 Glyceraldehyde 3-phosphate dehydrogenase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	337	Total	C	N	O	S	0	10	0
			2576	1620	447	495	14			
1	A	337	Total	C	N	O	S	0	4	0
			2557	1608	446	490	13			
1	B	337	Total	C	N	O	S	0	4	0
			2555	1607	445	490	13			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	188	ALA	SER	ENGINEERED	UNP P19866
A	188	ALA	SER	ENGINEERED	UNP P19866
B	188	ALA	SER	ENGINEERED	UNP P19866

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
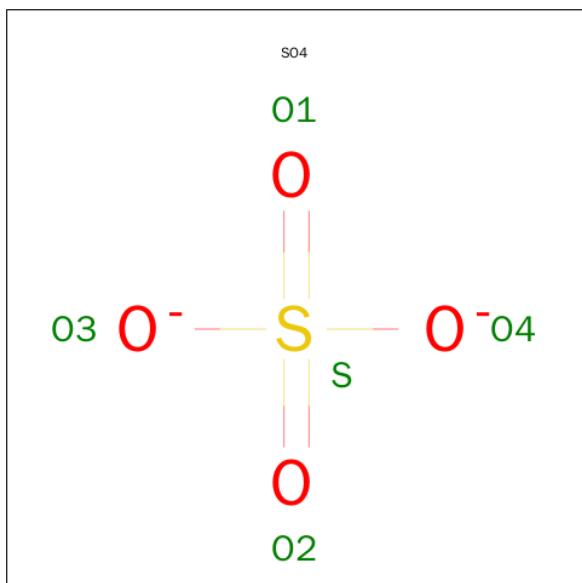
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	O	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).
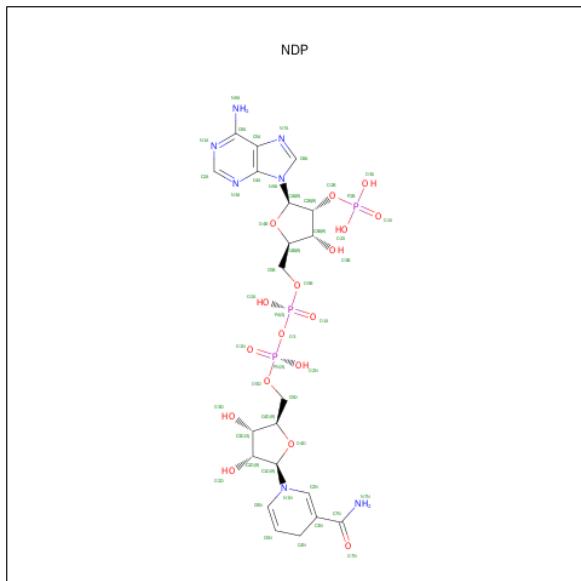
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	O	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	134	Total	O	0	0
			134	134		
4	B	133	Total	O	0	0
			133	133		
4	O	214	Total	O	0	0
			214	214		

3 Residue-property plots ⓘ

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: Glyceraldehyde 3-phosphate dehydrogenase A
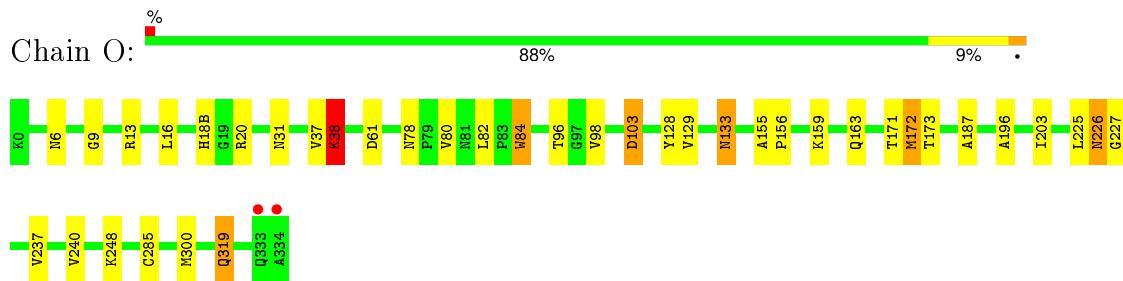
- Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase A
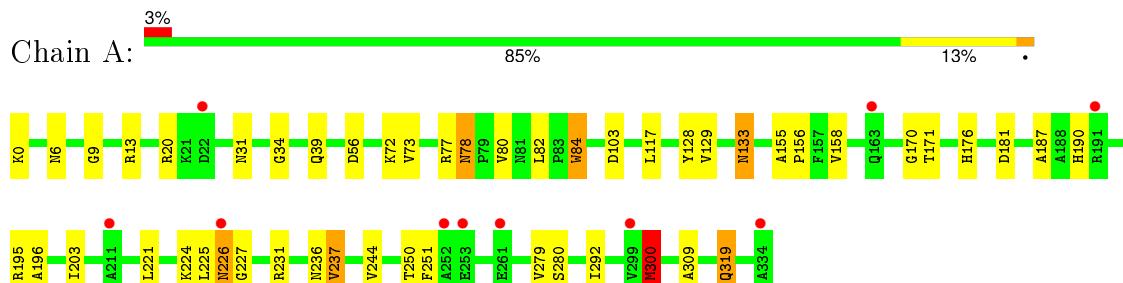
- Molecule 1: Glyceraldehyde 3-phosphate dehydrogenase A
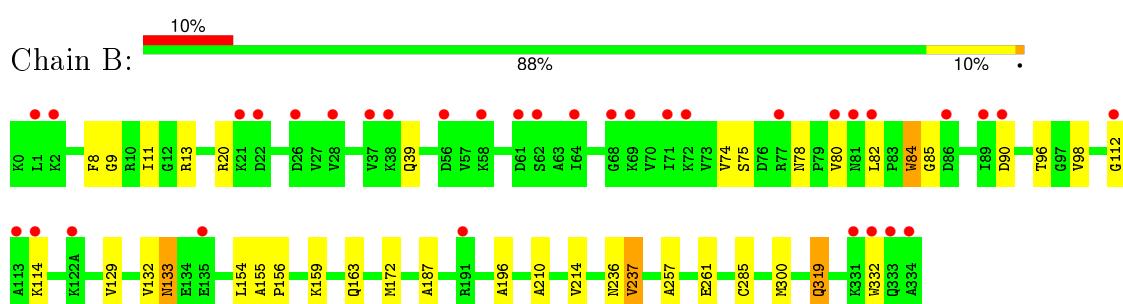
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	143.90Å 190.29Å 109.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	79.06 – 2.10 95.15 – 2.10	Depositor EDS
% Data completeness (in resolution range)	97.7 (79.06-2.10) 97.9 (95.15-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	7.24 (at 2.10Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.224 , 0.254 0.225 , 0.257	Depositor DCC
R_{free} test set	4336 reflections (5.08%)	DCC
Wilson B-factor (Å^2)	25.3	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 62.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 85405 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8363	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NDP, 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	0.39	0/2614	0.65	5/3548 (0.1%)
1	B	0.38	0/2612	0.65	2/3545 (0.1%)
1	O	0.55	0/2657	0.77	7/3604 (0.2%)
All	All	0.45	0/7883	0.69	14/10697 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	38[A]	LYS	CB-CA-C	-6.06	98.28	110.40
1	O	38[B]	LYS	CB-CA-C	-6.06	98.28	110.40
1	O	300[A]	MET	CB-CA-C	-6.00	98.39	110.40
1	O	300[B]	MET	CB-CA-C	-6.00	98.39	110.40
1	A	300[A]	MET	CB-CA-C	-5.93	98.54	110.40
1	A	300[B]	MET	CB-CA-C	-5.93	98.54	110.40
1	O	203	ILE	N-CA-C	-5.31	96.67	111.00
1	O	103[A]	ASP	CB-CA-C	-5.22	99.95	110.40
1	O	103[B]	ASP	CB-CA-C	-5.22	99.95	110.40
1	A	203	ILE	N-CA-C	-5.13	97.16	111.00
1	A	56[A]	ASP	N-CA-CB	5.05	119.69	110.60
1	A	56[B]	ASP	N-CA-CB	5.05	119.69	110.60
1	B	300[A]	MET	N-CA-CB	5.02	119.63	110.60
1	B	300[B]	MET	N-CA-CB	5.02	119.63	110.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2557	0	2586	47	0
1	B	2555	0	2585	26	0
1	O	2576	0	2605	33	0
2	A	20	0	0	0	0
2	B	15	0	0	0	0
2	O	15	0	0	0	0
3	A	48	0	26	0	0
3	B	48	0	26	1	0
3	O	48	0	26	0	0
4	A	134	0	0	2	0
4	B	133	0	0	0	0
4	O	214	0	0	2	0
All	All	8363	0	7854	105	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 7.

All (105) 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:O:6:ASN:HD21	1:O:31:ASN:HD22	1.26	0.82
1:O:37:VAL:HG13	1:O:38[B]:LYS:HD2	1.62	0.78
1:A:78:ASN:ND2	1:A:80:VAL:HG12	2.00	0.77
1:O:6:ASN:ND2	1:O:31:ASN:HD22	1.83	0.76
1:A:170:GLY:HA3	1:A:244:VAL:HG12	1.68	0.76
1:O:78:ASN:OD1	1:O:80:VAL:HG22	1.88	0.73
1:A:6:ASN:ND2	1:A:31:ASN:HD22	1.88	0.72
1:A:171:THR:HA	1:A:226[B]:ASN:ND2	2.04	0.72
1:O:172[A]:MET:HG2	1:O:173:THR:N	2.05	0.72
1:A:6:ASN:HD21	1:A:31:ASN:HD22	1.36	0.71
1:A:155:ALA:HB3	1:A:156:PRO:HD3	1.71	0.71
1:B:78:ASN:OD1	1:B:80:VAL:HG22	1.91	0.70
1:O:20:ARG:HH21	1:O:319:GLN:NE2	1.92	0.66
1:A:171:THR:CB	1:A:226[B]:ASN:HD21	2.09	0.66
1:A:20:ARG:HH21	1:A:319:GLN:NE2	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LYS:C	1:A:225:LEU:HD12	2.18	0.64
1:B:20:ARG:HH11	1:B:319:GLN:HE22	1.46	0.63
1:B:319:GLN:HA	1:B:319:GLN:HE21	1.64	0.63
1:A:171:THR:HA	1:A:226[B]:ASN:HD21	1.65	0.61
1:A:82:LEU:HD13	1:A:84:TRP:CZ2	2.36	0.61
1:B:129:VAL:H	1:B:133:ASN:HD21	1.48	0.60
1:O:172[A]:MET:HG2	1:O:173:THR:H	1.65	0.60
1:O:37:VAL:HG13	1:O:38[B]:LYS:CD	2.32	0.59
1:A:0:LYS:HB3	1:A:0:LYS:NZ	2.18	0.59
1:O:319:GLN:HE21	1:O:319:GLN:HA	1.68	0.58
1:O:159:LYS:O	1:O:163:GLN:HG3	2.04	0.58
1:A:171:THR:CA	1:A:226[B]:ASN:HD21	2.17	0.57
1:B:20:ARG:HH11	1:B:319:GLN:NE2	2.01	0.57
1:B:155:ALA:HB3	1:B:156:PRO:HD3	1.86	0.57
1:A:78:ASN:HD21	1:A:80:VAL:HG12	1.70	0.56
1:A:158:VAL:CG1	1:A:221:LEU:HD21	2.36	0.56
1:O:172[A]:MET:HG3	1:O:240:VAL:HG13	1.87	0.56
1:O:96:THR:OG1	1:O:98:VAL:HG22	2.05	0.56
1:B:210:ALA:O	1:B:214:VAL:HG23	2.06	0.56
1:A:190:HIS:H	1:B:39:GLN:NE2	2.04	0.55
1:A:319:GLN:HA	1:A:319:GLN:HE21	1.72	0.55
1:B:90:ASP:HA	1:B:114:LYS:HD2	1.89	0.55
1:O:18(B):HIS:HD2	4:O:7519:HOH:O	1.89	0.54
1:B:129:VAL:H	1:B:133:ASN:ND2	2.05	0.53
1:B:82:LEU:HD13	1:B:84:TRP:CZ2	2.44	0.53
1:B:96:THR:OG1	1:B:98:VAL:HG22	2.09	0.53
1:B:74:VAL:HG12	1:B:75:SER:N	2.25	0.52
1:O:155:ALA:HB3	1:O:156:PRO:HD3	1.92	0.51
1:A:34:GLY:HA3	1:A:39:GLN:OE1	2.12	0.50
1:O:20:ARG:HH21	1:O:319:GLN:HE21	1.60	0.50
1:B:84:TRP:HE3	1:B:84:TRP:HA	1.77	0.49
1:A:236:ASN:O	1:A:237:VAL:HB	2.11	0.49
1:O:129:VAL:H	1:O:133:ASN:HD21	1.59	0.49
1:B:20:ARG:NH1	1:B:319:GLN:NE2	2.60	0.49
1:B:84:TRP:CE3	1:B:84:TRP:HA	2.47	0.49
1:A:20:ARG:HH21	1:A:319:GLN:HE21	1.59	0.48
1:A:0:LYS:HB3	1:A:0:LYS:HZ3	1.78	0.48
1:B:11:ILE:HD11	3:B:2335:NDP:H42N	1.96	0.47
1:A:226[A]:ASN:ND2	1:A:227:GLY:H	2.13	0.47
1:O:129:VAL:H	1:O:133:ASN:ND2	2.12	0.47
1:A:279:VAL:HG22	1:A:280:SER:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:LEU:HD12	1:A:221:LEU:N	2.30	0.46
1:O:171:THR:CB	1:O:226[A]:ASN:HD21	2.28	0.46
1:O:20:ARG:HE	1:O:319:GLN:HE22	1.64	0.46
1:B:187:ALA:O	1:B:196:ALA:HB1	2.15	0.46
1:O:128:TYR:HA	1:O:133:ASN:HD21	1.81	0.46
1:A:129:VAL:H	1:A:133:ASN:HD21	1.62	0.46
1:A:176:HIS:HB3	1:A:231:ARG:HD3	1.97	0.45
1:A:129:VAL:H	1:A:133:ASN:ND2	2.14	0.45
1:O:82:LEU:HD13	1:O:84:TRP:CZ2	2.52	0.45
1:O:226[B]:ASN:ND2	1:O:227:GLY:H	2.14	0.45
1:B:236:ASN:O	1:B:237:VAL:HB	2.17	0.45
1:A:9:GLY:O	1:A:13:ARG:HG3	2.17	0.44
1:A:187:ALA:O	1:A:196:ALA:HB1	2.18	0.44
1:A:225:LEU:N	1:A:225:LEU:HD12	2.33	0.44
1:A:250:THR:OG1	1:A:251:PHE:N	2.51	0.44
1:O:226[B]:ASN:HD22	1:O:227:GLY:H	1.65	0.43
1:B:85:GLY:CA	1:B:112:GLY:HA3	2.48	0.43
1:B:132:VAL:HG21	1:B:155:ALA:HB1	2.01	0.43
1:A:128:TYR:HA	1:A:133:ASN:HD21	1.83	0.43
1:O:248:LYS:HE3	4:O:7485:HOH:O	2.19	0.43
1:A:78:ASN:C	1:A:78:ASN:HD22	2.22	0.43
1:O:171:THR:HA	1:O:226[A]:ASN:ND2	2.34	0.43
1:O:9:GLY:O	1:O:13:ARG:HG3	2.19	0.43
1:A:171:THR:HB	1:A:226[B]:ASN:HD21	1.81	0.42
1:A:72:LYS:HG3	1:A:73:VAL:N	2.33	0.42
1:B:90:ASP:O	1:B:114:LYS:HB2	2.20	0.42
1:B:154:LEU:HD11	1:B:172:MET:SD	2.60	0.41
1:A:158:VAL:HG12	1:A:221:LEU:HD21	2.02	0.41
1:A:181:ASP:OD2	1:A:195:ARG:NH1	2.42	0.41
1:B:9:GLY:O	1:B:13:ARG:HG3	2.20	0.41
1:A:117:LEU:C	1:A:117:LEU:HD23	2.40	0.41
1:A:103:ASP:HB2	4:A:1420:HOH:O	2.19	0.41
1:A:221:LEU:N	1:A:221:LEU:CD1	2.84	0.41
1:A:292:ILE:HD13	1:A:309:ALA:HB2	2.02	0.41
1:A:251:PHE:CD1	1:A:251:PHE:N	2.89	0.41
1:B:159:LYS:O	1:B:163:GLN:HG3	2.21	0.41
1:A:77:ARG:HG2	4:A:1426:HOH:O	2.21	0.41
1:A:279:VAL:HG22	1:A:280:SER:H	1.86	0.40
1:O:187:ALA:O	1:O:196:ALA:HB1	2.21	0.40
1:B:257:ALA:O	1:B:261:GLU:HG3	2.22	0.40
1:O:16:LEU:O	1:O:16:LEU:HD13	2.21	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	339/337 (101%)	316 (93%)	22 (6%)	1 (0%)	46	45
1	B	339/337 (101%)	316 (93%)	22 (6%)	1 (0%)	46	45
1	O	345/337 (102%)	328 (95%)	16 (5%)	1 (0%)	46	45
All	All	1023/1011 (101%)	960 (94%)	60 (6%)	3 (0%)	46	45

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	O	237	VAL
1	A	237	VAL
1	B	237	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	282/278 (101%)	274 (97%)	8 (3%)	51	55
1	B	282/278 (101%)	276 (98%)	6 (2%)	61	66
1	O	288/278 (104%)	274 (95%)	14 (5%)	31	28
All	All	852/834 (102%)	824 (97%)	28 (3%)	54	47

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	38[A]	LYS
1	O	38[B]	LYS
1	O	61	ASP
1	O	84	TRP
1	O	103[A]	ASP
1	O	103[B]	ASP
1	O	133	ASN
1	O	172[A]	MET
1	O	172[B]	MET
1	O	225	LEU
1	O	226[A]	ASN
1	O	226[B]	ASN
1	O	285	CYS
1	O	319	GLN
1	A	78	ASN
1	A	84	TRP
1	A	133	ASN
1	A	226[A]	ASN
1	A	226[B]	ASN
1	A	300[A]	MET
1	A	300[B]	MET
1	A	319	GLN
1	B	8	PHE
1	B	84	TRP
1	B	133	ASN
1	B	285	CYS
1	B	319	GLN
1	B	332	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	6	ASN
1	O	18(B)	HIS
1	O	81	ASN
1	O	133	ASN
1	O	152	ASN
1	O	220	ASN
1	O	256	ASN
1	O	265	ASN
1	O	319	GLN
1	A	6	ASN
1	A	14	ASN

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Mol	Chain	Res	Type
1	A	78	ASN
1	A	81	ASN
1	A	133	ASN
1	A	152	ASN
1	A	256	ASN
1	A	265	ASN
1	A	319	GLN
1	A	330	ASN
1	B	6	ASN
1	B	14	ASN
1	B	39	GLN
1	B	133	ASN
1	B	152	ASN
1	B	256	ASN
1	B	265	ASN
1	B	319	GLN
1	B	330	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

13 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
3	NDP	A	1335	-	42,52,52	1.36	4 (9%)	55,80,80	2.27	12 (21%)
2	SO4	A	1338	-	4,4,4	0.17	0	6,6,6	0.07	0
2	SO4	A	1339	-	4,4,4	0.21	0	6,6,6	0.07	0
2	SO4	A	901	-	4,4,4	0.19	0	6,6,6	0.09	0
2	SO4	A	903	-	4,4,4	0.19	0	6,6,6	0.09	0
3	NDP	B	2335	-	42,52,52	1.35	4 (9%)	55,80,80	2.25	12 (21%)
2	SO4	B	2338	-	4,4,4	0.17	0	6,6,6	0.08	0
2	SO4	B	2339	-	4,4,4	0.21	0	6,6,6	0.09	0
2	SO4	B	904	-	4,4,4	0.19	0	6,6,6	0.08	0
3	NDP	O	7335	-	42,52,52	1.36	4 (9%)	55,80,80	2.29	13 (23%)
2	SO4	O	7338	-	4,4,4	0.12	0	6,6,6	0.09	0
2	SO4	O	7339	-	4,4,4	0.23	0	6,6,6	0.06	0
2	SO4	O	902	-	4,4,4	0.24	0	6,6,6	0.14	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	NDP	A	1335	-	-	0/30/77/77	0/5/5/5
2	SO4	A	1338	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1339	-	-	0/0/0/0	0/0/0/0
2	SO4	A	901	-	-	0/0/0/0	0/0/0/0
2	SO4	A	903	-	-	0/0/0/0	0/0/0/0
3	NDP	B	2335	-	-	0/30/77/77	0/5/5/5
2	SO4	B	2338	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2339	-	-	0/0/0/0	0/0/0/0
2	SO4	B	904	-	-	0/0/0/0	0/0/0/0
3	NDP	O	7335	-	-	0/30/77/77	0/5/5/5
2	SO4	O	7338	-	-	0/0/0/0	0/0/0/0
2	SO4	O	7339	-	-	0/0/0/0	0/0/0/0
2	SO4	O	902	-	-	0/0/0/0	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1335	NDP	C4N-C5N	-4.41	1.39	1.49
3	O	7335	NDP	C4N-C5N	-4.36	1.39	1.49
3	B	2335	NDP	C4N-C5N	-4.32	1.39	1.49
3	B	2335	NDP	C2N-C3N	2.72	1.41	1.34
3	O	7335	NDP	C2N-C3N	2.73	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1335	NDP	C2N-C3N	2.77	1.41	1.34
3	B	2335	NDP	C6N-C5N	3.47	1.40	1.33
3	O	7335	NDP	C6N-C5N	3.49	1.40	1.33
3	A	1335	NDP	C6N-C5N	3.49	1.40	1.33
3	A	1335	NDP	P2B-O1X	3.69	1.63	1.51
3	B	2335	NDP	P2B-O1X	3.69	1.63	1.51
3	O	7335	NDP	P2B-O1X	3.69	1.63	1.51

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	O	7335	NDP	N3A-C2A-N1A	-8.78	122.17	128.89
3	A	1335	NDP	N3A-C2A-N1A	-8.73	122.21	128.89
3	O	7335	NDP	C4B-O4B-C1B	-8.66	100.20	109.72
3	A	1335	NDP	C4B-O4B-C1B	-8.62	100.25	109.72
3	B	2335	NDP	C4B-O4B-C1B	-8.57	100.30	109.72
3	B	2335	NDP	N3A-C2A-N1A	-8.57	122.33	128.89
3	O	7335	NDP	O3D-C3D-C4D	-2.79	102.69	111.05
3	A	1335	NDP	O3D-C3D-C4D	-2.78	102.73	111.05
3	B	2335	NDP	O3D-C3D-C4D	-2.76	102.77	111.05
3	A	1335	NDP	O2X-P2B-O1X	-2.61	102.17	110.58
3	B	2335	NDP	O2X-P2B-O1X	-2.60	102.21	110.58
3	O	7335	NDP	O2X-P2B-O1X	-2.60	102.22	110.58
3	O	7335	NDP	O5D-PN-O1N	-2.46	100.08	109.62
3	B	2335	NDP	O5D-PN-O1N	-2.45	100.10	109.62
3	A	1335	NDP	O5D-PN-O1N	-2.44	100.13	109.62
3	O	7335	NDP	C1D-N1N-C6N	-2.24	115.79	120.81
3	A	1335	NDP	C1D-N1N-C6N	-2.21	115.87	120.81
3	B	2335	NDP	C1D-N1N-C6N	-2.18	115.93	120.81
3	O	7335	NDP	C1B-N9A-C4A	-2.16	123.68	126.94
3	B	2335	NDP	C3N-C2N-N1N	-2.14	120.07	123.14
3	O	7335	NDP	C3N-C2N-N1N	-2.12	120.10	123.14
3	B	2335	NDP	C1B-N9A-C4A	-2.12	123.75	126.94
3	A	1335	NDP	P2B-O2B-C2B	-2.08	116.57	121.56
3	A	1335	NDP	C1B-N9A-C4A	-2.08	123.80	126.94
3	A	1335	NDP	C3N-C2N-N1N	-2.06	120.19	123.14
3	B	2335	NDP	P2B-O2B-C2B	-2.03	116.69	121.56
3	O	7335	NDP	P2B-O2B-C2B	-2.02	116.73	121.56
3	O	7335	NDP	C2D-C1D-N1N	2.58	120.31	113.34
3	B	2335	NDP	C5N-C4N-C3N	2.78	120.19	112.52
3	O	7335	NDP	C5N-C4N-C3N	2.79	120.22	112.52
3	A	1335	NDP	C5N-C4N-C3N	2.79	120.22	112.52

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Mol	Chain	Res	Type	Atoms	Z	Observed($^\circ$)	Ideal($^\circ$)
3	O	7335	NDP	O3X-P2B-O2X	3.78	121.76	107.38
3	A	1335	NDP	O3X-P2B-O2X	3.81	121.90	107.38
3	B	2335	NDP	O3X-P2B-O2X	3.82	121.93	107.38
3	B	2335	NDP	C4A-C5A-N7A	4.84	113.93	109.48
3	A	1335	NDP	C4A-C5A-N7A	4.89	113.97	109.48
3	O	7335	NDP	C4A-C5A-N7A	4.89	113.98	109.48

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
3	B	2335	NDP	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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	337/337 (100%)	0.08	10 (2%)	54	62	19, 32, 49, 58	0
1	B	337/337 (100%)	0.40	34 (10%)	9	12	16, 35, 67, 87	0
1	O	337/337 (100%)	-0.02	2 (0%)	90	92	9, 20, 34, 55	0
All	All	1011/1011 (100%)	0.15	46 (4%)	37	46	9, 28, 59, 87	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	334	ALA	8.3
1	O	334	ALA	6.8
1	B	332	TRP	6.5
1	A	334	ALA	5.9
1	B	333	GLN	5.1
1	B	38	LYS	4.3
1	B	69	LYS	4.3
1	B	61	ASP	4.1
1	B	62	SER	4.1
1	B	81	ASN	3.6
1	B	22	ASP	3.5
1	B	37	VAL	3.2
1	A	191	ARG	3.0
1	B	77	ARG	3.0
1	B	113	ALA	2.9
1	A	163	GLN	2.9
1	B	58	LYS	2.9
1	B	80	VAL	2.9
1	B	1	LEU	2.8
1	B	135	GLU	2.8
1	A	22	ASP	2.7
1	B	82	LEU	2.6
1	B	86	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	261	GLU	2.3
1	B	2	LYS	2.3
1	B	89	ILE	2.3
1	B	331	LYS	2.3
1	B	26	ASP	2.2
1	B	56[A]	ASP	2.2
1	B	68	GLY	2.2
1	B	114	LYS	2.2
1	A	299	VAL	2.2
1	B	71	ILE	2.2
1	B	112	GLY	2.2
1	B	72	LYS	2.2
1	O	333	GLN	2.1
1	B	21	LYS	2.1
1	B	122(A)	LYS	2.1
1	A	253	GLU	2.1
1	B	64	ILE	2.1
1	B	28	VAL	2.1
1	B	191	ARG	2.0
1	A	211	ALA	2.0
1	A	252	ALA	2.0
1	A	226[A]	ASN	2.0
1	B	90	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å²)	Q<0.9
2	SO4	B	2339	5/5	0.88	0.15	4.90	62,63,63,63	0
2	SO4	O	902	5/5	0.84	0.20	4.01	41,44,45,45	5
2	SO4	A	1339	5/5	0.88	0.15	2.60	62,63,64,64	0
3	NDP	A	1335	48/48	0.86	0.17	2.49	23,33,47,50	0
3	NDP	O	7335	48/48	0.90	0.14	1.11	15,24,44,49	0
3	NDP	B	2335	48/48	0.87	0.17	0.71	35,43,65,66	0
2	SO4	A	901	5/5	0.93	0.17	-0.13	56,57,57,58	5
2	SO4	O	7339	5/5	0.94	0.12	-0.19	59,59,59,60	0
2	SO4	O	7338	5/5	0.99	0.12	-	34,35,37,37	0
2	SO4	A	1338	5/5	0.96	0.14	-	63,64,64,64	0
2	SO4	A	903	5/5	0.85	0.23	-	70,70,71,71	5
2	SO4	B	2338	5/5	0.97	0.14	-	61,61,62,62	0
2	SO4	B	904	5/5	0.88	0.23	-	84,84,84,84	5

6.5 Other polymers (i)

There are no such residues in this entry.