



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:20 AM UTC

PDB ID : 1QI6 / pdb_00001qi6
Title : SECOND APO FORM OF AN NADP DEPENDENT ALDEHYDE DEHYDROGENASE WITH GLU250 SITUATED 3.7 Å FROM CYS284
Authors : Cobessi, D.; Tete-Favier, F.; Marchal, S.; Branlant, G.; Aubry, A.
Deposited on : 1999-06-02
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

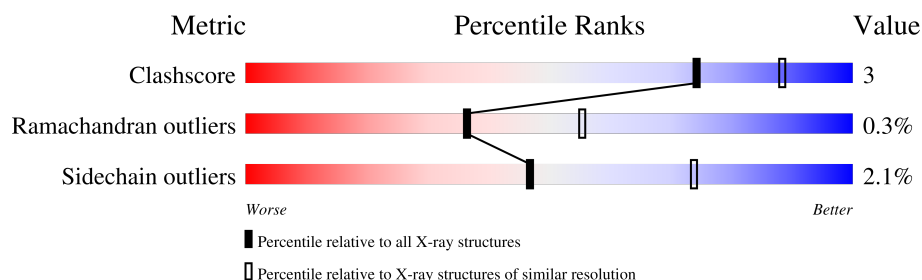
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	475	
1	B	475	
1	C	475	
1	D	475	

2 Entry composition [i](#)

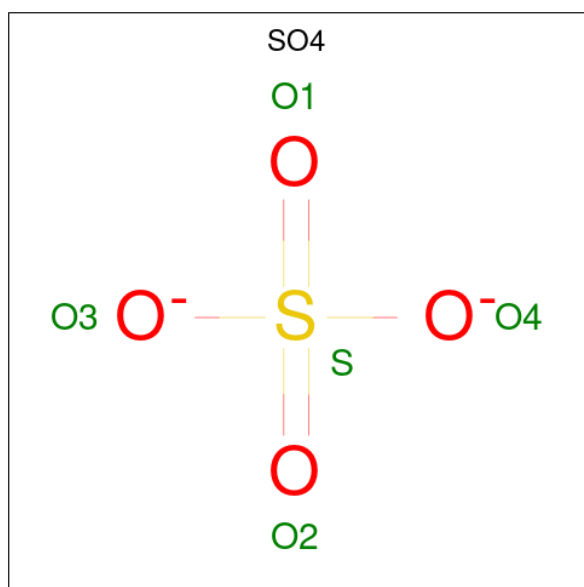
There are 3 unique types of molecules in this entry. The entry contains 15009 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (NADP DEPENDENT NONPHOSPHORYLATING GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	474	Total	C	N	O	S	0	0	0
			3596	2286	600	699	11			
1	B	474	Total	C	N	O	S	0	0	0
			3596	2286	600	699	11			
1	C	474	Total	C	N	O	S	0	0	0
			3596	2286	600	699	11			
1	D	474	Total	C	N	O	S	0	0	0
			3596	2286	600	699	11			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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

- Molecule 3 is water.

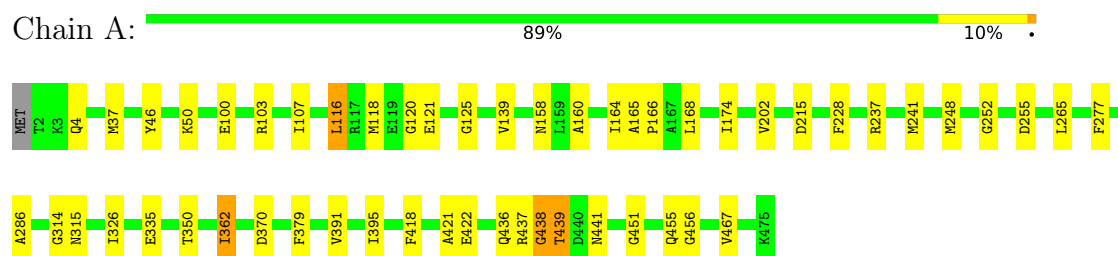
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	131	Total	O	0	0
			131	131		
3	B	147	Total	O	0	0
			147	147		
3	C	143	Total	O	0	0
			143	143		
3	D	144	Total	O	0	0
			144	144		

3 Residue-property plots [i](#)

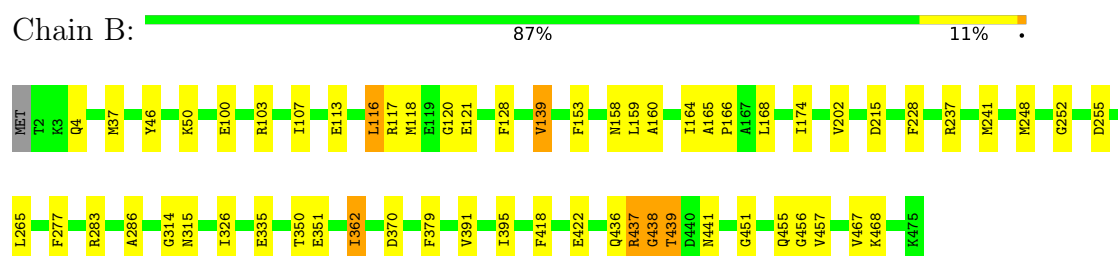
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

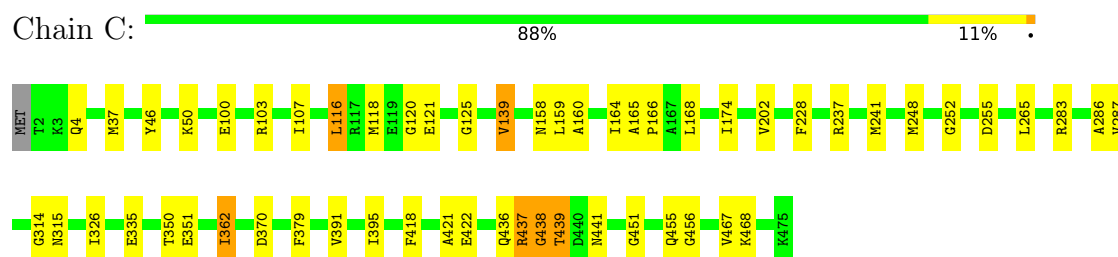
- Molecule 1: PROTEIN (NADP DEPENDENT NONPHOSPHORYLATING GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE)



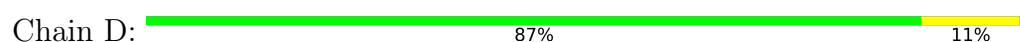
- Molecule 1: PROTEIN (NADP DEPENDENT NONPHOSPHORYLATING GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE)

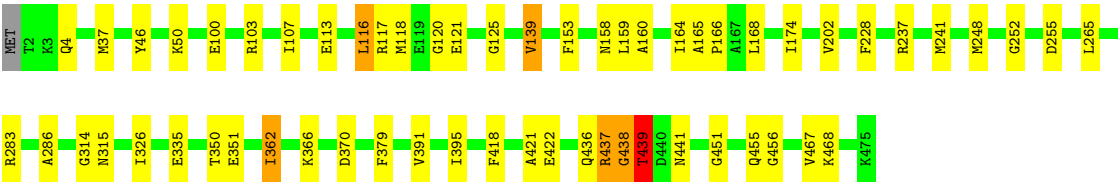


- Molecule 1: PROTEIN (NADP DEPENDENT NONPHOSPHORYLATING GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE)



- Molecule 1: PROTEIN (NADP DEPENDENT NONPHOSPHORYLATING GLYCERALDEHYDE-3-PHOSPHATE DEHYDROGENASE)





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	140.80Å 157.50Å 110.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	96.0 (8.00-2.50)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.232 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15009	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.46	0/3654	0.95	18/4942 (0.4%)
1	B	0.47	0/3654	0.95	20/4942 (0.4%)
1	C	0.48	0/3654	0.95	20/4942 (0.4%)
1	D	0.47	0/3654	0.96	20/4942 (0.4%)
All	All	0.47	0/14616	0.95	78/19768 (0.4%)

There are no bond length outliers.

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	456	GLY	N-CA-C	-9.62	99.12	111.72
1	D	456	GLY	N-CA-C	-9.28	99.56	111.72
1	A	456	GLY	N-CA-C	-9.24	99.61	111.72
1	D	160	ALA	N-CA-C	-8.04	102.43	112.72
1	B	160	ALA	N-CA-C	-8.01	102.47	112.72
1	C	160	ALA	N-CA-C	-7.77	102.60	112.93
1	A	160	ALA	N-CA-C	-7.73	102.65	112.93
1	D	174	ILE	N-CA-C	7.10	118.70	108.48
1	A	174	ILE	N-CA-C	7.06	118.65	108.48
1	B	174	ILE	N-CA-C	7.00	118.55	108.48
1	C	174	ILE	N-CA-C	6.99	118.54	108.48
1	B	37	MET	N-CA-C	6.20	118.30	110.24
1	A	451	GLY	N-CA-C	6.10	119.04	110.38
1	B	326	ILE	N-CA-C	6.07	117.54	110.62
1	D	326	ILE	N-CA-C	6.04	117.50	110.62
1	B	265	LEU	N-CA-C	6.03	118.65	111.71
1	A	326	ILE	N-CA-C	6.02	117.48	110.62
1	C	451	GLY	N-CA-C	6.01	118.92	110.38
1	A	265	LEU	N-CA-C	6.01	118.62	111.71
1	D	265	LEU	N-CA-C	5.99	118.60	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	265	LEU	N-CA-C	5.94	118.54	111.71
1	C	326	ILE	N-CA-C	5.94	117.39	110.62
1	A	362	ILE	N-CA-C	5.84	117.09	108.45
1	A	37	MET	N-CA-C	5.74	117.69	110.24
1	D	315	ASN	CA-C-N	5.72	125.40	119.05
1	D	315	ASN	C-N-CA	5.72	125.40	119.05
1	B	437	ARG	N-CA-C	-5.71	106.17	113.01
1	A	315	ASN	CA-C-N	5.69	125.36	119.05
1	A	315	ASN	C-N-CA	5.69	125.36	119.05
1	D	362	ILE	N-CA-C	5.66	116.82	108.45
1	D	37	MET	N-CA-C	5.65	118.03	110.35
1	D	437	ARG	N-CA-C	-5.63	106.26	113.01
1	D	164	ILE	N-CA-C	5.61	115.74	110.30
1	B	451	GLY	N-CA-C	5.60	118.64	110.63
1	B	252	GLY	N-CA-C	5.59	119.74	112.25
1	B	164	ILE	N-CA-C	5.58	115.78	110.42
1	B	362	ILE	N-CA-C	5.58	116.70	108.45
1	C	168	LEU	N-CA-C	5.58	117.44	111.36
1	D	451	GLY	N-CA-C	5.57	118.59	110.63
1	B	315	ASN	CA-C-N	5.55	125.64	119.32
1	B	315	ASN	C-N-CA	5.55	125.64	119.32
1	B	139	VAL	N-CA-C	5.52	115.81	107.80
1	D	139	VAL	N-CA-C	5.49	115.76	107.80
1	C	37	MET	N-CA-C	5.49	117.81	110.35
1	A	437	ARG	N-CA-C	-5.48	106.44	113.01
1	A	164	ILE	N-CA-C	5.43	115.63	110.42
1	A	228	PHE	N-CA-C	5.40	117.60	109.23
1	B	228	PHE	N-CA-C	5.39	117.58	109.23
1	C	164	ILE	N-CA-C	5.38	115.52	110.30
1	C	362	ILE	N-CA-C	5.38	116.41	108.45
1	B	4	GLN	N-CA-C	5.36	117.47	108.96
1	D	228	PHE	N-CA-C	5.34	117.50	109.23
1	D	252	GLY	N-CA-C	5.33	119.39	112.25
1	C	252	GLY	N-CA-C	5.26	119.30	112.25
1	C	228	PHE	N-CA-C	5.25	117.37	109.23
1	D	4	GLN	N-CA-C	5.25	117.31	108.96
1	C	437	ARG	N-CA-C	-5.25	106.72	113.01
1	D	351	GLU	N-CA-C	5.23	117.46	110.35
1	A	168	LEU	N-CA-C	5.21	117.04	111.36
1	A	252	GLY	N-CA-C	5.20	119.21	112.25
1	D	168	LEU	N-CA-C	5.19	117.02	111.36
1	C	315	ASN	N-CA-C	5.18	117.44	110.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	456	GLY	N-CA-C	-5.18	99.43	111.04
1	C	4	GLN	N-CA-C	5.18	117.19	108.96
1	B	277	PHE	N-CA-C	5.15	119.66	113.17
1	B	314	GLY	N-CA-C	5.15	117.53	110.58
1	D	314	GLY	N-CA-C	5.13	117.51	110.58
1	B	168	LEU	N-CA-C	5.13	116.95	111.36
1	C	314	GLY	N-CA-C	5.11	117.47	110.58
1	A	314	GLY	N-CA-C	5.09	117.45	110.58
1	C	315	ASN	CA-C-N	5.08	125.11	119.32
1	C	315	ASN	C-N-CA	5.08	125.11	119.32
1	B	351	GLU	N-CA-C	5.07	117.24	110.35
1	A	277	PHE	N-CA-C	5.06	119.55	113.17
1	C	351	GLU	N-CA-C	5.05	117.21	110.35
1	A	4	GLN	N-CA-C	5.04	116.97	108.96
1	D	315	ASN	N-CA-C	5.03	117.59	110.24
1	C	139	VAL	N-CA-C	5.01	115.06	107.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3596	0	3649	22	0
1	B	3596	0	3649	26	0
1	C	3596	0	3649	24	0
1	D	3596	0	3649	28	0
2	A	15	0	0	0	0
2	B	15	0	0	0	0
2	C	15	0	0	0	0
2	D	15	0	0	1	0
3	A	131	0	0	0	0
3	B	147	0	0	0	0
3	C	143	0	0	1	0
3	D	144	0	0	1	0
All	All	15009	0	14596	89	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 3.

All (89) 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:D:436:GLN:HE21	1:D:438:GLY:HA3	1.40	0.86
1:B:436:GLN:HE21	1:B:438:GLY:HA3	1.40	0.86
1:A:436:GLN:HE21	1:A:438:GLY:HA3	1.41	0.84
1:C:436:GLN:HE21	1:C:438:GLY:HA3	1.42	0.83
1:A:237:ARG:HG2	1:A:241:MET:HE2	1.72	0.70
1:B:237:ARG:HG2	1:B:241:MET:HE2	1.75	0.67
1:D:237:ARG:HG2	1:D:241:MET:HE2	1.78	0.66
1:C:237:ARG:HG2	1:C:241:MET:HE2	1.76	0.66
1:A:165:ALA:HB3	1:A:166:PRO:HD3	1.81	0.62
1:B:100:GLU:HG3	1:B:158:ASN:HB2	1.82	0.61
1:A:100:GLU:HG3	1:A:158:ASN:HB2	1.83	0.60
1:C:125:GLY:HA2	1:D:439:THR:HG21	1.83	0.60
1:D:100:GLU:HG3	1:D:158:ASN:HB2	1.82	0.60
1:C:100:GLU:HG3	1:C:158:ASN:HB2	1.82	0.60
1:C:165:ALA:HB3	1:C:166:PRO:HD3	1.85	0.59
1:A:125:GLY:HA2	1:B:439:THR:HG21	1.85	0.58
1:D:165:ALA:HB3	1:D:166:PRO:HD3	1.86	0.57
1:B:165:ALA:HB3	1:B:166:PRO:HD3	1.85	0.57
1:C:439:THR:HG22	1:C:441:ASN:OD1	2.06	0.56
1:C:350:THR:OG1	1:C:362:ILE:HA	2.07	0.55
1:A:350:THR:OG1	1:A:362:ILE:HA	2.07	0.54
1:C:46:TYR:O	1:C:50:LYS:HG2	2.08	0.54
1:B:350:THR:OG1	1:B:362:ILE:HA	2.08	0.54
1:A:439:THR:HG22	1:A:441:ASN:OD1	2.08	0.54
1:D:350:THR:OG1	1:D:362:ILE:HA	2.09	0.53
1:A:46:TYR:O	1:A:50:LYS:HG2	2.09	0.52
1:D:46:TYR:O	1:D:50:LYS:HG2	2.10	0.52
1:D:439:THR:HG22	1:D:441:ASN:OD1	2.08	0.52
1:B:439:THR:HG22	1:B:441:ASN:OD1	2.09	0.52
1:C:436:GLN:NE2	1:C:438:GLY:HA3	2.20	0.52
1:A:255:ASP:HB2	1:A:286:ALA:O	2.09	0.52
1:B:46:TYR:O	1:B:50:LYS:HG2	2.10	0.51
1:C:255:ASP:HB2	1:C:286:ALA:O	2.10	0.51
1:A:248:MET:SD	1:A:455:GLN:HG3	2.51	0.50
1:D:436:GLN:NE2	1:D:438:GLY:HA3	2.18	0.50
1:D:366:LYS:HG3	3:D:727:HOH:O	2.13	0.49
1:B:436:GLN:NE2	1:B:438:GLY:HA3	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:ASP:HB2	1:B:286:ALA:O	2.13	0.49
1:A:421:ALA:O	1:B:468:LYS:HE2	2.13	0.48
1:D:255:ASP:HB2	1:D:286:ALA:O	2.14	0.48
1:B:248:MET:SD	1:B:455:GLN:HG3	2.53	0.47
1:D:248:MET:SD	1:D:455:GLN:HG3	2.53	0.47
1:C:248:MET:SD	1:C:455:GLN:HG3	2.54	0.47
1:A:436:GLN:NE2	1:A:438:GLY:HA3	2.20	0.46
1:A:107:ILE:HD12	1:A:158:ASN:HD21	1.82	0.45
1:C:120:GLY:HA3	1:C:139:VAL:O	2.17	0.45
1:C:391:VAL:O	1:C:395:ILE:HG13	2.17	0.45
1:C:421:ALA:O	1:D:468:LYS:HE2	2.17	0.45
1:C:439:THR:HG21	1:D:125:GLY:HA2	1.98	0.45
1:B:103:ARG:O	1:B:107:ILE:HG13	2.16	0.44
1:C:287:VAL:HG23	3:C:607:HOH:O	2.17	0.44
1:D:107:ILE:HD12	1:D:158:ASN:HD21	1.81	0.44
1:D:418:PHE:O	1:D:422:GLU:HG3	2.17	0.44
1:C:107:ILE:HD12	1:C:158:ASN:HD21	1.82	0.44
1:A:120:GLY:HA3	1:A:139:VAL:O	2.18	0.44
1:B:107:ILE:HD12	1:B:158:ASN:HD21	1.83	0.44
1:A:116:LEU:HD12	1:A:116:LEU:C	2.43	0.43
1:A:439:THR:HG22	1:B:128:PHE:HB3	2.01	0.43
1:C:103:ARG:O	1:C:107:ILE:HG13	2.18	0.43
1:A:103:ARG:O	1:A:107:ILE:HG13	2.19	0.43
1:D:103:ARG:O	1:D:107:ILE:HG13	2.19	0.43
1:A:215:ASP:OD2	1:A:237:ARG:NH2	2.52	0.42
1:C:116:LEU:C	1:C:116:LEU:HD12	2.44	0.42
1:D:120:GLY:HA3	1:D:139:VAL:O	2.19	0.42
1:D:283:ARG:HH21	1:D:437:ARG:NH1	2.17	0.42
1:A:391:VAL:O	1:A:395:ILE:HG13	2.19	0.42
1:D:116:LEU:HD12	1:D:116:LEU:C	2.44	0.42
1:B:117:ARG:NH2	1:D:113:GLU:HB2	2.34	0.42
1:B:121:GLU:HA	1:C:121:GLU:HA	2.00	0.42
1:B:418:PHE:O	1:B:422:GLU:HG3	2.20	0.42
1:A:418:PHE:O	1:A:422:GLU:HG3	2.20	0.42
1:D:391:VAL:O	1:D:395:ILE:HG13	2.19	0.42
1:D:437:ARG:NH1	2:D:587:SO4:O4	2.53	0.42
1:B:113:GLU:HB2	1:D:117:ARG:NH2	2.34	0.42
1:C:418:PHE:O	1:C:422:GLU:HG3	2.20	0.42
1:D:159:LEU:HD23	1:D:159:LEU:HA	1.90	0.42
1:B:283:ARG:HH21	1:B:437:ARG:NH1	2.19	0.41
1:C:159:LEU:HD23	1:C:159:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:LEU:HD23	1:B:159:LEU:HA	1.88	0.41
1:D:153:PHE:CD1	1:D:153:PHE:C	2.98	0.41
1:C:283:ARG:HH21	1:C:437:ARG:NH1	2.18	0.41
1:A:107:ILE:HD12	1:A:158:ASN:ND2	2.36	0.41
1:B:153:PHE:CD1	1:B:153:PHE:C	2.99	0.40
1:B:215:ASP:OD2	1:B:237:ARG:NH2	2.54	0.40
1:B:116:LEU:C	1:B:116:LEU:HD12	2.46	0.40
1:B:120:GLY:HA3	1:B:139:VAL:O	2.19	0.40
1:A:121:GLU:HA	1:D:121:GLU:HA	2.04	0.40
1:B:391:VAL:O	1:B:395:ILE:HG13	2.22	0.40
1:C:468:LYS:HE2	1:D:421:ALA:O	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	472/475 (99%)	454 (96%)	17 (4%)	1 (0%)	43	63
1	B	472/475 (99%)	453 (96%)	17 (4%)	2 (0%)	30	49
1	C	472/475 (99%)	452 (96%)	19 (4%)	1 (0%)	43	63
1	D	472/475 (99%)	453 (96%)	17 (4%)	2 (0%)	30	49
All	All	1888/1900 (99%)	1812 (96%)	70 (4%)	6 (0%)	36	55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	438	GLY
1	B	438	GLY
1	C	438	GLY
1	D	438	GLY

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Mol	Chain	Res	Type
1	D	439	THR
1	B	457	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	378/379 (100%)	370 (98%)	8 (2%)	47	74
1	B	378/379 (100%)	370 (98%)	8 (2%)	47	74
1	C	378/379 (100%)	370 (98%)	8 (2%)	47	74
1	D	378/379 (100%)	370 (98%)	8 (2%)	47	74
All	All	1512/1516 (100%)	1480 (98%)	32 (2%)	47	74

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	LEU
1	A	118	MET
1	A	202	VAL
1	A	335	GLU
1	A	370	ASP
1	A	379	PHE
1	A	439	THR
1	A	467	VAL
1	B	116	LEU
1	B	118	MET
1	B	202	VAL
1	B	335	GLU
1	B	370	ASP
1	B	379	PHE
1	B	439	THR
1	B	467	VAL
1	C	116	LEU
1	C	118	MET
1	C	202	VAL

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Mol	Chain	Res	Type
1	C	335	GLU
1	C	370	ASP
1	C	379	PHE
1	C	439	THR
1	C	467	VAL
1	D	116	LEU
1	D	118	MET
1	D	202	VAL
1	D	335	GLU
1	D	370	ASP
1	D	379	PHE
1	D	439	THR
1	D	467	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	158	ASN
1	A	221	GLN
1	A	315	ASN
1	A	436	GLN
1	A	455	GLN
1	B	18	ASN
1	B	158	ASN
1	B	221	GLN
1	B	315	ASN
1	B	436	GLN
1	B	455	GLN
1	C	158	ASN
1	C	271	ASN
1	C	315	ASN
1	C	436	GLN
1	C	455	GLN
1	D	158	ASN
1	D	271	ASN
1	D	315	ASN
1	D	436	GLN
1	D	455	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	SO4	C	582	-	4,4,4	0.34	0	6,6,6	0.16	0
2	SO4	B	580	-	4,4,4	0.36	0	6,6,6	0.08	0
2	SO4	D	586	-	4,4,4	0.36	0	6,6,6	0.14	0
2	SO4	A	577	-	4,4,4	0.35	0	6,6,6	0.06	0
2	SO4	C	584	-	4,4,4	0.30	0	6,6,6	0.18	0
2	SO4	C	583	-	4,4,4	0.33	0	6,6,6	0.09	0
2	SO4	A	578	-	4,4,4	0.32	0	6,6,6	0.08	0
2	SO4	D	585	-	4,4,4	0.36	0	6,6,6	0.14	0
2	SO4	A	576	-	4,4,4	0.34	0	6,6,6	0.18	0
2	SO4	B	579	-	4,4,4	0.36	0	6,6,6	0.08	0
2	SO4	D	587	-	4,4,4	0.37	0	6,6,6	0.11	0
2	SO4	B	581	-	4,4,4	0.35	0	6,6,6	0.14	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	D	587	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.