Full wwPDB X-ray Structure Validation Report (i)

May 3, 2022 – 02:17 PM EDT

PDB ID	:	6NA3
Title	:	Crystal Structure of Apo-form of ECR
Authors	:	DeMirci, H.
Deposited on	:	2018-12-05
Resolution	:	1.80 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 following versions of software and data (see references (1)) were used in the production of this report:

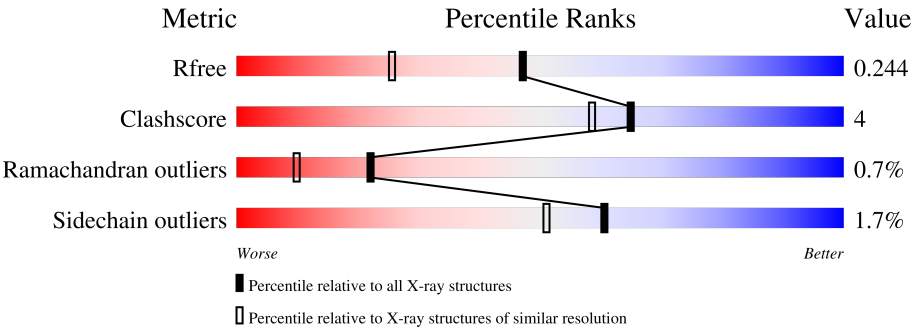
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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%

Mol	Chain	Length	Quality of chain
1	A	445	92% 7% •
1	B	445	91% 8% •
1	C	445	90% 9% •
1	D	445	89% 10% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15205 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.

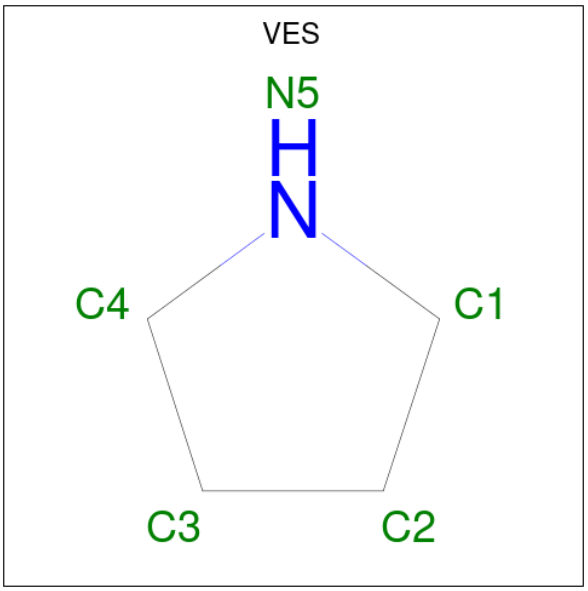
- Molecule 1 is a protein called Putative crotonyl-CoA reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	445	Total	C	N	O	S	6	2	0
			3449	2169	621	646	13			
1	B	445	Total	C	N	O	S	0	1	0
			3448	2169	623	643	13			
1	C	445	Total	C	N	O	S	0	1	0
			3448	2169	623	643	13			
1	D	444	Total	C	N	O	S	0	2	0
			3446	2168	620	645	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ARG	-	expression tag	UNP E4N096
A	0	HIS	-	expression tag	UNP E4N096
B	-1	ARG	-	expression tag	UNP E4N096
B	0	HIS	-	expression tag	UNP E4N096
C	-1	ARG	-	expression tag	UNP E4N096
C	0	HIS	-	expression tag	UNP E4N096
D	-1	ARG	-	expression tag	UNP E4N096
D	0	HIS	-	expression tag	UNP E4N096

- Molecule 2 is Pyrrolidine (three-letter code: VES) (formula: C_4H_9N).



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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is water.

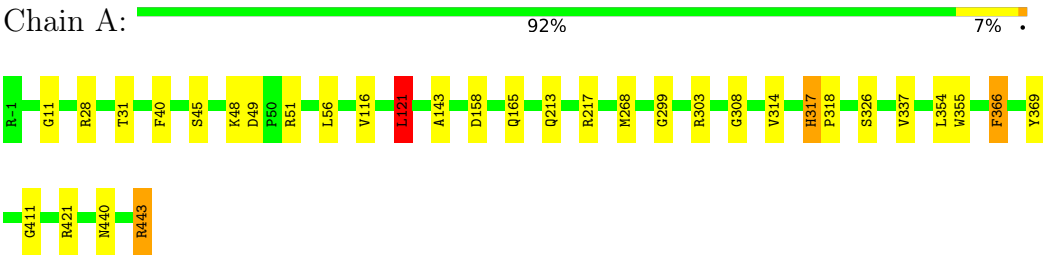
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	311	Total O 312 312	0	1
4	B	365	Total O 367 367	0	2
4	C	316	Total O 318 318	0	2
4	D	368	Total O 372 372	0	4

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.

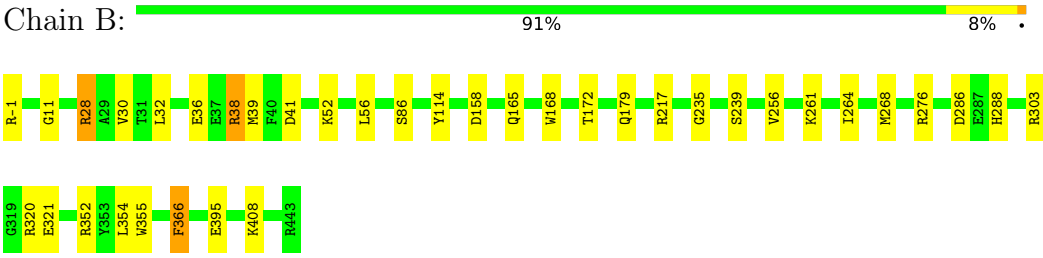
• Molecule 1: Putative crotonyl-CoA reductase

Chain A:



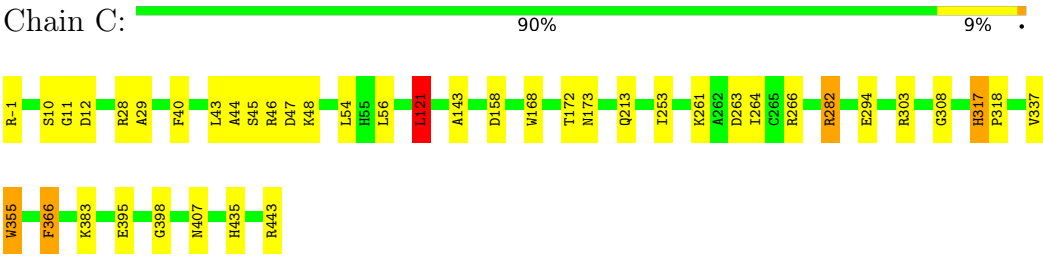
• Molecule 1: Putative crotonyl-CoA reductase

Chain B:



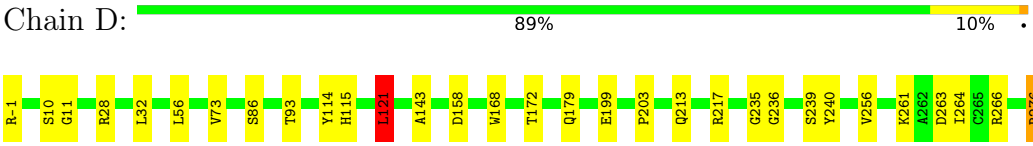
• Molecule 1: Putative crotonyl-CoA reductase

Chain C:



• Molecule 1: Putative crotonyl-CoA reductase

Chain D:




H289
G299
R303
G308
H317
P318
V337
L354
W355
R360
F366
K390
V391
Y392
L402
L418
K438
F442
ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.10Å 153.00Å 202.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	16.97 – 1.80 48.11 – 1.37	Depositor EDS
% Data completeness (in resolution range)	91.3 (16.97-1.80) 80.3 (48.11-1.37)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.05 (at 1.37Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.199 , 0.242 0.203 , 0.244	Depositor DCC
R_{free} test set	2000 reflections (0.49%)	wwPDB-VP
Wilson B-factor (Å^2)	14.4	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 51.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.57$, $< L^2 > = 0.42$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15205	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.16 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.9510e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: VES, CL

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	0.49	0/3531	0.67	3/4787 (0.1%)
1	B	0.51	0/3530	0.69	2/4785 (0.0%)
1	C	0.47	0/3530	0.70	2/4785 (0.0%)
1	D	0.51	0/3528	0.72	6/4783 (0.1%)
All	All	0.49	0/14119	0.69	13/19140 (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	B	0	1
1	C	0	1
1	D	0	1
All	All	0	4

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	366	PHE	N-CA-CB	-7.03	97.95	110.60
1	A	121	LEU	CA-CB-CG	6.85	131.06	115.30
1	B	366	PHE	N-CA-CB	-6.75	98.45	110.60
1	D	10	SER	C-N-CA	-6.60	108.43	122.30
1	D	121	LEU	CB-CG-CD2	6.34	121.78	111.00
1	D	418	LEU	CA-CB-CG	6.32	129.83	115.30
1	A	56	LEU	CA-CB-CG	-6.28	100.86	115.30
1	C	121	LEU	CA-CB-CG	6.22	129.60	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	366	PHE	N-CA-CB	-6.02	99.77	110.60
1	D	360	ARG	CA-CB-CG	5.50	125.51	113.40
1	D	121	LEU	CA-CB-CG	5.45	127.84	115.30
1	A	366	PHE	N-CA-CB	-5.29	101.08	110.60
1	B	366	PHE	CB-CA-C	-5.08	100.23	110.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	11	GLY	Peptide
1	B	11	GLY	Peptide
1	C	11	GLY	Peptide
1	D	11	GLY	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	3449	0	3379	21	0
1	B	3448	0	3383	28	0
1	C	3448	0	3383	31	0
1	D	3446	0	3375	29	0
2	A	10	0	18	1	0
2	B	15	0	27	4	0
2	C	5	0	9	0	0
2	D	10	0	18	3	0
3	A	2	0	0	1	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	312	0	0	4	0
4	B	367	0	0	6	0
4	C	318	0	0	5	1
4	D	372	0	0	4	1
All	All	15205	0	13592	111	1

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 4.

All (111) 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)
3:A:504:CL:CL	4:A:803:HOH:O	2.23	0.91
1:C:43:LEU:HD21	1:C:47:ASP:HB2	1.64	0.79
1:A:45:SER:HA	1:A:48:LYS:HD2	1.65	0.78
1:B:56:LEU:HD11	1:B:395:GLU:HA	1.65	0.76
1:D:286:ASP:HB3	1:D:288:HIS:H	1.51	0.75
1:B:320[A]:ARG:NH1	4:B:603:HOH:O	2.20	0.74
1:A:217:ARG:HG2	2:B:501:VES:H21C	1.69	0.73
1:B:321:GLU:OE2	4:B:601:HOH:O	2.08	0.70
1:A:40:PHE:HB3	1:A:48:LYS:HE2	1.73	0.68
1:C:45:SER:HA	1:C:48:LYS:HD2	1.74	0.68
1:A:443:ARG:NH1	4:A:601:HOH:O	2.27	0.67
1:C:-1:ARG:NH1	4:C:601:HOH:O	2.19	0.67
1:C:263:ASP:OD1	1:C:266:ARG:NH1	2.28	0.66
1:D:317:HIS:H	1:D:318:PRO:CD	2.09	0.66
1:D:263:ASP:OD1	1:D:266:ARG:NH1	2.29	0.66
1:C:56:LEU:HD12	1:C:395:GLU:HA	1.78	0.66
1:A:303:ARG:NH1	4:A:602:HOH:O	2.30	0.65
1:B:317:HIS:H	1:B:318:PRO:CD	2.10	0.64
1:A:440:ASN:O	1:A:443:ARG:HG3	1.98	0.64
1:C:317:HIS:H	1:C:318:PRO:HD3	1.63	0.63
1:A:317:HIS:H	1:A:318:PRO:CD	2.12	0.63
1:A:299:GLY:O	1:A:303:ARG:HG3	1.98	0.62
1:C:443:ARG:NE	1:C:443:ARG:HA	2.15	0.62
1:C:43:LEU:CD2	1:C:47:ASP:HB2	2.30	0.62
1:A:317:HIS:H	1:A:318:PRO:HD3	1.65	0.61
1:C:317:HIS:H	1:C:318:PRO:CD	2.13	0.61
2:D:502:VES:H32C	4:D:603:HOH:O	2.01	0.60
1:C:56:LEU:CD1	1:C:395:GLU:HA	2.31	0.60
1:B:317:HIS:H	1:B:318:PRO:HD3	1.65	0.60
1:D:317:HIS:H	1:D:318:PRO:HD3	1.66	0.59
1:D:276[B]:ARG:NH1	4:D:607:HOH:O	2.38	0.57
1:C:29:ALA:O	1:C:56:LEU:HD23	2.06	0.56
1:C:303:ARG:HB3	1:C:308:GLY:HA2	1.85	0.56
1:B:276:ARG:NH1	4:B:609:HOH:O	2.39	0.56
1:C:54:LEU:HD12	1:C:398:GLY:HA2	1.88	0.56
1:A:49:ASP:OD2	1:A:51:ARG:NH2	2.31	0.56
1:C:43:LEU:HD21	1:C:47:ASP:CB	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:ARG:NH2	4:B:607:HOH:O	2.33	0.54
1:B:286:ASP:HB3	1:B:288:HIS:H	1.72	0.54
1:B:56:LEU:CD1	1:B:395:GLU:HA	2.37	0.53
1:C:40:PHE:CG	1:C:48:LYS:HG2	2.43	0.53
1:B:165:GLN:NE2	4:B:610:HOH:O	2.41	0.53
1:D:168:TRP:HD1	1:D:172:THR:HG21	1.74	0.53
1:A:268:MET:HA	2:A:501:VES:H22C	1.90	0.52
1:D:-1:ARG:N	4:D:609:HOH:O	2.43	0.52
1:B:36:GLU:HB3	1:B:39:MET:HE2	1.91	0.51
1:C:-1:ARG:HG2	4:C:646:HOH:O	2.10	0.51
1:C:168:TRP:HD1	1:C:172:THR:HG21	1.75	0.51
1:A:303:ARG:HB3	1:A:308:GLY:HA2	1.91	0.51
1:D:438:LYS:NZ	4:D:603:HOH:O	2.30	0.51
1:B:268:MET:HG2	2:B:502:VES:H21C	1.93	0.50
1:D:217:ARG:CZ	2:D:501:VES:H31C	2.41	0.50
1:C:261:LYS:HA	1:C:264:ILE:HD12	1.93	0.50
1:B:168:TRP:HD1	1:B:172:THR:HG21	1.76	0.50
1:A:314:VAL:HG11	1:A:326:SER:HB3	1.94	0.49
1:D:235:GLY:O	1:D:239:SER:HB3	2.12	0.49
1:A:121:LEU:HD22	1:A:143:ALA:HB2	1.94	0.49
1:C:43:LEU:HD23	1:C:44:ALA:N	2.28	0.49
1:D:73:VAL:O	1:D:418:LEU:HB2	2.13	0.49
1:B:28:ARG:H	1:B:179:GLN:NE2	2.11	0.48
1:B:32:LEU:HD21	1:B:86:SER:HA	1.94	0.48
1:D:303:ARG:HB3	1:D:308:GLY:HA2	1.95	0.48
1:B:261:LYS:HA	1:B:264:ILE:HD12	1.95	0.48
1:D:286:ASP:HB2	1:D:289:HIS:H	1.79	0.48
1:B:30:VAL:HG22	1:B:56:LEU:HD21	1.96	0.48
1:A:213:GLN:HG3	1:A:337:VAL:HG22	1.94	0.48
1:C:351:ASN:ND2	1:C:355:TRP:HE3	2.13	0.47
1:D:56:LEU:HD12	1:D:56:LEU:HA	1.69	0.47
1:B:38:ARG:HD3	1:B:41:ASP:OD2	2.15	0.47
1:A:165:GLN:NE2	4:C:829[B]:HOH:O	2.47	0.46
1:A:51:ARG:HE	1:A:51:ARG:HB2	1.61	0.46
1:C:282:ARG:O	1:C:294:GLU:HG3	2.15	0.46
1:B:52:LYS:HD2	1:B:52:LYS:N	2.29	0.46
1:C:213:GLN:HG3	1:C:337:VAL:HG22	1.98	0.46
1:B:217:ARG:HG2	2:B:501:VES:H11C	1.96	0.46
1:A:389:SER:HB3	1:A:411:GLY:HA3	1.97	0.46
1:A:31:THR:HG22	1:A:116:VAL:HG22	1.98	0.45
1:D:93:THR:HG21	1:D:115:HIS:ND1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:213:GLN:HG3	1:D:337:VAL:HG22	1.98	0.45
1:B:-1:ARG:HG3	4:B:701:HOH:O	2.16	0.45
1:B:352:ARG:HD2	2:B:503:VES:H42C	1.99	0.45
1:C:121:LEU:HD22	1:C:143:ALA:HB2	1.99	0.45
1:D:179:GLN:HB3	1:D:418:LEU:HD13	1.98	0.45
1:B:28:ARG:H	1:B:179:GLN:HE21	1.66	0.44
1:D:236:GLY:O	1:D:240:TYR:HD2	2.00	0.44
1:B:235:GLY:O	1:B:239:SER:HB3	2.18	0.43
1:C:317:HIS:N	1:C:318:PRO:CD	2.82	0.42
1:C:40:PHE:HB3	1:C:48:LYS:HE2	2.01	0.42
1:C:383:LYS:HA	1:C:383:LYS:HD3	1.89	0.42
1:D:217:ARG:NE	2:D:501:VES:H31C	2.34	0.42
1:D:199:GLU:O	1:D:203:PRO:HD3	2.19	0.42
1:C:12:ASP:OD1	1:C:12:ASP:N	2.52	0.42
1:C:172:THR:HG22	1:C:173:ASN:O	2.20	0.42
1:D:121:LEU:HD22	1:D:143:ALA:HB2	2.00	0.42
1:C:253:ILE:HD12	1:C:253:ILE:N	2.35	0.42
1:D:261:LYS:HA	1:D:264:ILE:HD12	2.01	0.42
1:C:435:HIS:HE1	4:C:740:HOH:O	2.02	0.41
1:A:317:HIS:N	1:A:318:PRO:CD	2.80	0.41
1:D:32:LEU:O	1:D:114:TYR:HA	2.20	0.41
1:A:421:ARG:NE	4:A:604:HOH:O	2.31	0.41
1:D:256:VAL:O	1:D:276[A]:ARG:HG2	2.21	0.41
1:D:402:LEU:HD23	1:D:402:LEU:HA	1.82	0.41
1:B:256:VAL:O	1:B:276:ARG:HG2	2.20	0.41
1:C:407:ASN:HA	4:C:754:HOH:O	2.20	0.41
1:B:408:LYS:HB2	1:B:408:LYS:HE3	1.88	0.41
1:D:32:LEU:HD21	1:D:86:SER:HA	2.02	0.41
1:D:317:HIS:N	1:D:318:PRO:CD	2.81	0.41
1:D:299:GLY:O	1:D:303:ARG:HG3	2.21	0.41
1:D:390:LYS:HD3	1:D:392:TYR:CE2	2.55	0.40
1:B:286:ASP:CB	1:B:288:HIS:H	2.33	0.40
1:B:32:LEU:O	1:B:114:TYR:HA	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:869:HOH:O	4:D:941:HOH:O[2_454]	2.09	0.11

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	445/445 (100%)	433 (97%)	9 (2%)	3 (1%)	22	10
1	B	444/445 (100%)	434 (98%)	7 (2%)	3 (1%)	22	10
1	C	444/445 (100%)	431 (97%)	10 (2%)	3 (1%)	22	10
1	D	444/445 (100%)	433 (98%)	8 (2%)	3 (1%)	22	10
All	All	1777/1780 (100%)	1731 (97%)	34 (2%)	12 (1%)	22	10

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	HIS
1	A	366	PHE
1	B	317	HIS
1	B	366	PHE
1	C	317	HIS
1	C	366	PHE
1	D	317	HIS
1	D	366	PHE
1	A	158	ASP
1	B	158	ASP
1	C	158	ASP
1	D	158	ASP

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	359/357 (101%)	352 (98%)	7 (2%)	57 46
1	B	358/357 (100%)	353 (99%)	5 (1%)	67 59
1	C	358/357 (100%)	351 (98%)	7 (2%)	55 44
1	D	358/357 (100%)	352 (98%)	6 (2%)	60 51
All	All	1433/1428 (100%)	1408 (98%)	25 (2%)	60 51

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ARG
1	A	121	LEU
1	A	354	LEU
1	A	355	TRP
1	A	369	TYR
1	A	407	ASN
1	A	443	ARG
1	B	28	ARG
1	B	38	ARG
1	B	316	GLU
1	B	354	LEU
1	B	355	TRP
1	C	10	SER
1	C	28	ARG
1	C	46	ARG
1	C	121	LEU
1	C	282	ARG
1	C	354	LEU
1	C	355	TRP
1	D	28	ARG
1	D	121	LEU
1	D	276[A]	ARG
1	D	276[B]	ARG
1	D	354	LEU
1	D	355	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	165	GLN
1	A	365	HIS

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Mol	Chain	Res	Type
1	B	179	GLN
1	C	435	HIS
1	D	289	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 5 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	VES	B	503	-	5,5,5	0.26	0	5,5,5	1.57	1 (20%)
2	VES	D	501	-	5,5,5	0.50	0	5,5,5	1.94	2 (40%)
2	VES	C	501	-	5,5,5	0.22	0	5,5,5	1.75	1 (20%)
2	VES	A	502	-	5,5,5	0.19	0	5,5,5	1.64	1 (20%)
2	VES	D	502	-	5,5,5	0.23	0	5,5,5	1.52	1 (20%)
2	VES	B	501	-	5,5,5	0.30	0	5,5,5	1.87	2 (40%)
2	VES	B	502	-	5,5,5	0.29	0	5,5,5	1.49	1 (20%)
2	VES	A	501	-	5,5,5	0.34	0	5,5,5	1.59	1 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	VES	B	503	-	-	-	0/1/1/1
2	VES	D	501	-	-	-	0/1/1/1
2	VES	C	501	-	-	-	0/1/1/1
2	VES	A	502	-	-	-	0/1/1/1
2	VES	D	502	-	-	-	0/1/1/1
2	VES	B	501	-	-	-	0/1/1/1
2	VES	B	502	-	-	-	0/1/1/1
2	VES	A	501	-	-	-	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	502	VES	C1-N5-C4	3.24	112.19	104.96
2	C	501	VES	C1-N5-C4	3.23	112.17	104.96
2	D	501	VES	C1-N5-C4	3.18	112.05	104.96
2	A	501	VES	C1-N5-C4	3.15	111.99	104.96
2	B	503	VES	C1-N5-C4	3.08	111.83	104.96
2	D	502	VES	C1-N5-C4	3.04	111.75	104.96
2	B	501	VES	C1-N5-C4	2.99	111.63	104.96
2	B	502	VES	C1-N5-C4	2.87	111.36	104.96
2	D	501	VES	C3-C2-C1	2.41	109.72	104.91
2	B	501	VES	C3-C2-C1	2.32	109.53	104.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	503	VES	1	0
2	D	501	VES	2	0
2	D	502	VES	1	0
2	B	501	VES	2	0
2	B	502	VES	1	0
2	A	501	VES	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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.