



Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 09:25 pm BST

PDB ID : 1ZSV
Title : Crystal structure of human NADP-dependent leukotriene B4 12-hydroxydehydrogenase
Authors : Turnbull, A.P.; Johansson, C.; Savitsky, P.; Guo, K.; Edwards, A.; Arrow-smith, C.; Sundstrom, M.; von Delft, F.; Oppermann, U.; Structural Genomics Consortium (SGC)
Deposited on : 2005-05-25
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

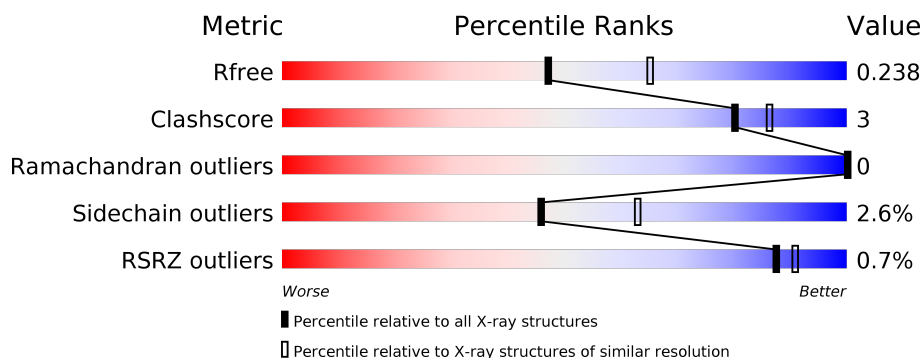
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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 $\leq 5\%$. 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	349	<div> <div>%</div> <div> <div></div> <div>85%</div> <div>8%</div> <div>6%</div> </div> </div>
1	B	349	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>6%</div> </div> </div>
1	C	349	<div> <div></div> <div> <div></div> <div>87%</div> <div>7%</div> <div>6%</div> </div> </div>
1	D	349	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>7%</div> <div>6%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	CL	A	407	-	-	X	-
2	CL	C	406	-	-	X	-
2	CL	D	401	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10171 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 NADP-dependent leukotriene B4 12-hydroxydehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2465	1597	399	454	15			
1	B	328	Total	C	N	O	S	0	0	0
			2450	1588	392	455	15			
1	C	328	Total	C	N	O	S	0	0	0
			2456	1591	398	452	15			
1	D	328	Total	C	N	O	S	0	0	0
			2463	1595	394	459	15			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	CLONING ARTIFACT	UNP Q14914
A	-18	HIS	-	EXPRESSION TAG	UNP Q14914
A	-17	HIS	-	EXPRESSION TAG	UNP Q14914
A	-16	HIS	-	EXPRESSION TAG	UNP Q14914
A	-15	HIS	-	EXPRESSION TAG	UNP Q14914
A	-14	HIS	-	EXPRESSION TAG	UNP Q14914
A	-13	HIS	-	EXPRESSION TAG	UNP Q14914
A	-12	SER	-	CLONING ARTIFACT	UNP Q14914
A	-11	SER	-	CLONING ARTIFACT	UNP Q14914
A	-10	GLY	-	CLONING ARTIFACT	UNP Q14914
A	-9	VAL	-	CLONING ARTIFACT	UNP Q14914
A	-8	ASP	-	CLONING ARTIFACT	UNP Q14914
A	-7	LEU	-	CLONING ARTIFACT	UNP Q14914
A	-6	GLY	-	CLONING ARTIFACT	UNP Q14914
A	-5	THR	-	CLONING ARTIFACT	UNP Q14914
A	-4	GLU	-	CLONING ARTIFACT	UNP Q14914
A	-3	ASN	-	CLONING ARTIFACT	UNP Q14914
A	-2	LEU	-	CLONING ARTIFACT	UNP Q14914
A	-1	TYR	-	CLONING ARTIFACT	UNP Q14914
A	0	PHE	-	CLONING ARTIFACT	UNP Q14914
A	1	GLN	-	CLONING ARTIFACT	UNP Q14914

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	-	CLONING ARTIFACT	UNP Q14914
A	3	MET	-	CLONING ARTIFACT	UNP Q14914
B	-19	MET	-	CLONING ARTIFACT	UNP Q14914
B	-18	HIS	-	EXPRESSION TAG	UNP Q14914
B	-17	HIS	-	EXPRESSION TAG	UNP Q14914
B	-16	HIS	-	EXPRESSION TAG	UNP Q14914
B	-15	HIS	-	EXPRESSION TAG	UNP Q14914
B	-14	HIS	-	EXPRESSION TAG	UNP Q14914
B	-13	HIS	-	EXPRESSION TAG	UNP Q14914
B	-12	SER	-	CLONING ARTIFACT	UNP Q14914
B	-11	SER	-	CLONING ARTIFACT	UNP Q14914
B	-10	GLY	-	CLONING ARTIFACT	UNP Q14914
B	-9	VAL	-	CLONING ARTIFACT	UNP Q14914
B	-8	ASP	-	CLONING ARTIFACT	UNP Q14914
B	-7	LEU	-	CLONING ARTIFACT	UNP Q14914
B	-6	GLY	-	CLONING ARTIFACT	UNP Q14914
B	-5	THR	-	CLONING ARTIFACT	UNP Q14914
B	-4	GLU	-	CLONING ARTIFACT	UNP Q14914
B	-3	ASN	-	CLONING ARTIFACT	UNP Q14914
B	-2	LEU	-	CLONING ARTIFACT	UNP Q14914
B	-1	TYR	-	CLONING ARTIFACT	UNP Q14914
B	0	PHE	-	CLONING ARTIFACT	UNP Q14914
B	1	GLN	-	CLONING ARTIFACT	UNP Q14914
B	2	SER	-	CLONING ARTIFACT	UNP Q14914
B	3	MET	-	CLONING ARTIFACT	UNP Q14914
C	-19	MET	-	CLONING ARTIFACT	UNP Q14914
C	-18	HIS	-	EXPRESSION TAG	UNP Q14914
C	-17	HIS	-	EXPRESSION TAG	UNP Q14914
C	-16	HIS	-	EXPRESSION TAG	UNP Q14914
C	-15	HIS	-	EXPRESSION TAG	UNP Q14914
C	-14	HIS	-	EXPRESSION TAG	UNP Q14914
C	-13	HIS	-	EXPRESSION TAG	UNP Q14914
C	-12	SER	-	CLONING ARTIFACT	UNP Q14914
C	-11	SER	-	CLONING ARTIFACT	UNP Q14914
C	-10	GLY	-	CLONING ARTIFACT	UNP Q14914
C	-9	VAL	-	CLONING ARTIFACT	UNP Q14914
C	-8	ASP	-	CLONING ARTIFACT	UNP Q14914
C	-7	LEU	-	CLONING ARTIFACT	UNP Q14914
C	-6	GLY	-	CLONING ARTIFACT	UNP Q14914
C	-5	THR	-	CLONING ARTIFACT	UNP Q14914
C	-4	GLU	-	CLONING ARTIFACT	UNP Q14914
C	-3	ASN	-	CLONING ARTIFACT	UNP Q14914

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	LEU	-	CLONING ARTIFACT	UNP Q14914
C	-1	TYR	-	CLONING ARTIFACT	UNP Q14914
C	0	PHE	-	CLONING ARTIFACT	UNP Q14914
C	1	GLN	-	CLONING ARTIFACT	UNP Q14914
C	2	SER	-	CLONING ARTIFACT	UNP Q14914
C	3	MET	-	CLONING ARTIFACT	UNP Q14914
D	-19	MET	-	CLONING ARTIFACT	UNP Q14914
D	-18	HIS	-	EXPRESSION TAG	UNP Q14914
D	-17	HIS	-	EXPRESSION TAG	UNP Q14914
D	-16	HIS	-	EXPRESSION TAG	UNP Q14914
D	-15	HIS	-	EXPRESSION TAG	UNP Q14914
D	-14	HIS	-	EXPRESSION TAG	UNP Q14914
D	-13	HIS	-	EXPRESSION TAG	UNP Q14914
D	-12	SER	-	CLONING ARTIFACT	UNP Q14914
D	-11	SER	-	CLONING ARTIFACT	UNP Q14914
D	-10	GLY	-	CLONING ARTIFACT	UNP Q14914
D	-9	VAL	-	CLONING ARTIFACT	UNP Q14914
D	-8	ASP	-	CLONING ARTIFACT	UNP Q14914
D	-7	LEU	-	CLONING ARTIFACT	UNP Q14914
D	-6	GLY	-	CLONING ARTIFACT	UNP Q14914
D	-5	THR	-	CLONING ARTIFACT	UNP Q14914
D	-4	GLU	-	CLONING ARTIFACT	UNP Q14914
D	-3	ASN	-	CLONING ARTIFACT	UNP Q14914
D	-2	LEU	-	CLONING ARTIFACT	UNP Q14914
D	-1	TYR	-	CLONING ARTIFACT	UNP Q14914
D	0	PHE	-	CLONING ARTIFACT	UNP Q14914
D	1	GLN	-	CLONING ARTIFACT	UNP Q14914
D	2	SER	-	CLONING ARTIFACT	UNP Q14914
D	3	MET	-	CLONING ARTIFACT	UNP Q14914

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	5	Total Cl 5 5	0	0
2	A	5	Total Cl 5 5	0	0
2	D	6	Total Cl 6 6	0	0
2	C	6	Total Cl 6 6	0	0

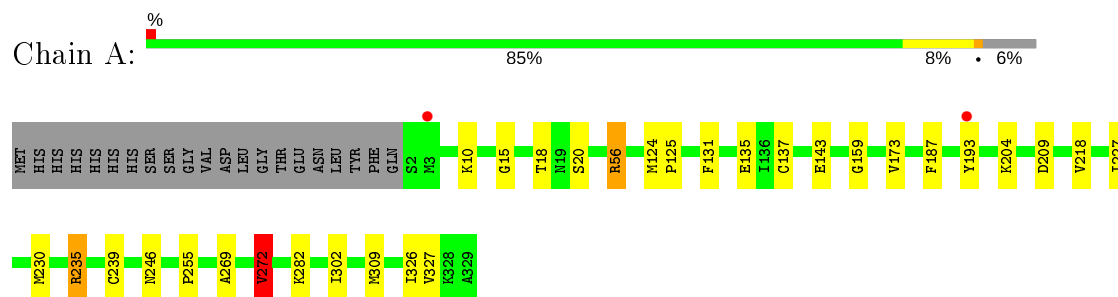
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	84	Total 84	O 84	0	0
3	B	71	Total 71	O 71	0	0
3	C	84	Total 84	O 84	0	0
3	D	76	Total 76	O 76	0	0

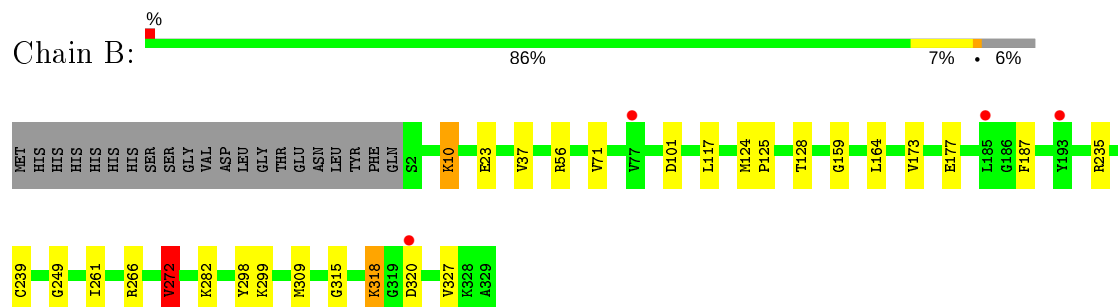
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

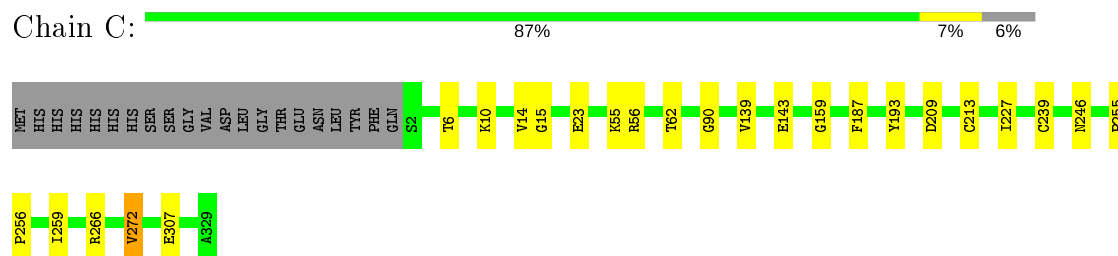
- Molecule 1: NADP-dependent leukotriene B4 12-hydroxydehydrogenase



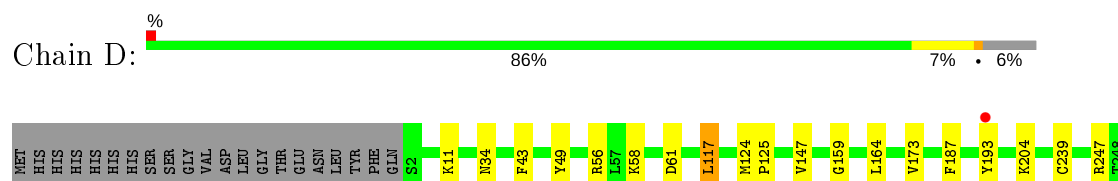
- Molecule 1: NADP-dependent leukotriene B4 12-hydroxydehydrogenase



- Molecule 1: NADP-dependent leukotriene B4 12-hydroxydehydrogenase



- Molecule 1: NADP-dependent leukotriene B4 12-hydroxydehydrogenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	92.54Å 92.54Å 202.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.30 – 2.30 62.28 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.4 (62.30-2.30) 98.4 (62.28-2.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.37 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.195 , 0.249 0.225 , 0.238	Depositor DCC
R_{free} test set	1917 reflections (2.58%)	wwPDB-VP
Wilson B-factor (Å ²)	40.9	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 24.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.468 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10171	wwPDB-VP
Average B, all atoms (Å ²)	46.0	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 40.35 % 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 2.7707e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: 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	0.83	1/2516 (0.0%)	0.85	4/3409 (0.1%)
1	B	0.82	1/2502 (0.0%)	0.80	4/3398 (0.1%)
1	C	0.82	1/2507 (0.0%)	0.82	2/3399 (0.1%)
1	D	0.82	1/2515 (0.0%)	0.80	2/3413 (0.1%)
All	All	0.82	4/10040 (0.0%)	0.82	12/13619 (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	D	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	239	CYS	CB-SG	-7.02	1.70	1.82
1	B	239	CYS	CB-SG	-6.92	1.70	1.82
1	A	239	CYS	CB-SG	-5.68	1.72	1.81
1	C	239	CYS	CB-SG	-5.40	1.73	1.81

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	A	235	ARG	NE-CZ-NH2	6.88	123.74	120.30
1	B	235	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	C	272	VAL	CB-CA-C	-6.62	98.82	111.40
1	D	56	ARG	NE-CZ-NH1	6.43	123.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	56	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	B	56	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	D	272	VAL	CB-CA-C	-5.68	100.61	111.40
1	A	272	VAL	CB-CA-C	-5.57	100.82	111.40
1	B	235	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	B	272	VAL	CB-CA-C	-5.40	101.14	111.40
1	A	235	ARG	NE-CZ-NH1	-5.33	117.64	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	249	GLY	Peptide

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	2465	0	2496	14	0
1	B	2450	0	2438	16	0
1	C	2456	0	2479	13	0
1	D	2463	0	2462	12	0
2	A	5	0	0	2	0
2	B	5	0	0	0	0
2	C	6	0	0	2	0
2	D	6	0	0	2	0
3	A	84	0	0	1	0
3	B	71	0	0	3	0
3	C	84	0	0	3	0
3	D	76	0	0	0	0
All	All	10171	0	9875	53	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 (53) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:GLY:HA3	3:C:503:HOH:O	1.90	0.72
1:A:193:TYR:CE2	2:A:407:CL:CL	2.81	0.71
1:C:193:TYR:CE2	2:C:406:CL:CL	2.91	0.60
1:C:90:GLY:O	3:C:485:HOH:O	2.16	0.59
1:D:159:GLY:HA3	1:D:187:PHE:CZ	2.38	0.59
1:D:302:ILE:HD13	1:D:326:ILE:HB	1.83	0.59
1:C:266:ARG:CD	3:C:447:HOH:O	2.52	0.57
1:D:193:TYR:CD2	2:D:401:CL:CL	2.96	0.55
1:B:266:ARG:CD	3:B:472:HOH:O	2.53	0.55
1:A:193:TYR:CD2	2:A:407:CL:CL	3.00	0.52
1:B:164:LEU:HD12	1:B:164:LEU:C	2.31	0.51
1:A:227:ILE:HD13	1:A:255:PRO:HB3	1.93	0.51
1:B:124:MET:HB3	1:B:125:PRO:HD3	1.94	0.50
1:C:6:THR:CG2	1:C:62:THR:HG23	2.42	0.49
1:A:159:GLY:HA3	1:A:187:PHE:CZ	2.47	0.49
1:A:302:ILE:HD13	1:A:326:ILE:HB	1.94	0.49
1:B:117:LEU:HD21	1:B:298:TYR:CD1	2.48	0.49
1:D:124:MET:HB3	1:D:125:PRO:HD3	1.96	0.48
1:A:309:MET:HG2	1:A:327:VAL:HG21	1.95	0.47
1:C:227:ILE:HD13	1:C:255:PRO:HB3	1.96	0.47
1:A:124:MET:HB3	1:A:125:PRO:HD3	1.97	0.47
1:C:193:TYR:CD2	2:C:406:CL:CL	3.05	0.47
1:C:256:PRO:HG2	1:C:259:ILE:HD12	1.97	0.46
1:D:164:LEU:HD12	1:D:164:LEU:O	2.15	0.46
1:B:159:GLY:HA3	1:B:187:PHE:CZ	2.51	0.46
1:C:10:LYS:HE2	1:C:23:GLU:HB2	1.98	0.46
1:B:299:LYS:NZ	3:B:459:HOH:O	2.48	0.45
1:B:177:GLU:HB2	3:B:455:HOH:O	2.17	0.45
1:C:159:GLY:HA3	1:C:187:PHE:CZ	2.52	0.45
1:C:139:VAL:HG12	1:C:213:CYS:SG	2.57	0.45
1:D:43:PHE:CE1	1:D:328:LYS:HG3	2.52	0.45
1:A:269:ALA:HB1	1:B:261:ILE:HA	1.99	0.45
1:A:272:VAL:HG22	3:A:442:HOH:O	2.16	0.44
1:B:128:THR:HA	1:B:272:VAL:HG13	1.99	0.44
1:B:10:LYS:HG3	1:B:23:GLU:HB2	2.00	0.44
1:B:318:LYS:HE3	1:C:14:VAL:HB	1.99	0.43
1:A:131:PHE:HD1	1:A:135:GLU:HG3	1.83	0.43
1:B:309:MET:HG3	1:B:327:VAL:HG21	2.00	0.43
1:A:10:LYS:HE2	1:A:20:SER:O	2.19	0.43
1:B:315:GLY:O	1:B:320:ASP:HB2	2.19	0.42
1:C:15:GLY:HA2	1:C:246:ASN:O	2.19	0.42
1:D:117:LEU:HD21	1:D:298:TYR:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ILE:HA	1:A:230:MET:HG2	2.01	0.42
1:D:58:LYS:O	1:D:61:ASP:HB2	2.19	0.42
1:B:101:ASP:N	1:B:101:ASP:OD1	2.53	0.42
1:A:15:GLY:HA2	1:A:246:ASN:O	2.20	0.41
1:B:37:VAL:HB	1:B:71:VAL:HG13	2.02	0.41
1:D:247:ARG:NH1	1:D:250:PRO:O	2.53	0.41
1:A:137:CYS:O	1:A:235:ARG:HD2	2.20	0.41
1:C:307:GLU:H	1:C:307:GLU:CD	2.23	0.40
1:D:43:PHE:HE1	1:D:328:LYS:HG3	1.86	0.40
1:D:49:TYR:C	1:D:49:TYR:CD1	2.94	0.40
1:D:193:TYR:CE2	2:D:401:CL:CL	3.12	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	326/349 (93%)	320 (98%)	6 (2%)	0	100	100
1	B	326/349 (93%)	321 (98%)	5 (2%)	0	100	100
1	C	326/349 (93%)	318 (98%)	8 (2%)	0	100	100
1	D	326/349 (93%)	319 (98%)	7 (2%)	0	100	100
All	All	1304/1396 (93%)	1278 (98%)	26 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	256/288 (89%)	247 (96%)	9 (4%)	36	50
1	B	250/288 (87%)	245 (98%)	5 (2%)	55	72
1	C	254/288 (88%)	250 (98%)	4 (2%)	62	78
1	D	254/288 (88%)	246 (97%)	8 (3%)	40	55
All	All	1014/1152 (88%)	988 (97%)	26 (3%)	46	63

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	THR
1	A	56	ARG
1	A	143	GLU
1	A	173	VAL
1	A	204	LYS
1	A	209	ASP
1	A	218	VAL
1	A	272	VAL
1	A	282	LYS
1	B	10	LYS
1	B	173	VAL
1	B	272	VAL
1	B	282	LYS
1	B	318	LYS
1	C	55	LYS
1	C	143	GLU
1	C	209	ASP
1	C	272	VAL
1	D	11	LYS
1	D	34	ASN
1	D	117	LEU
1	D	147	VAL
1	D	173	VAL
1	D	204	LYS
1	D	272	VAL
1	D	281	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	321	ASN
1	C	321	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](#)

Of 22 ligands modelled in this entry, 22 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	328/349 (93%)	0.03	2 (0%) 89 92	35, 46, 59, 70	0
1	B	328/349 (93%)	0.03	4 (1%) 79 83	37, 46, 59, 76	0
1	C	328/349 (93%)	0.00	0 100 100	36, 45, 59, 71	0
1	D	328/349 (93%)	0.04	3 (0%) 84 88	35, 46, 59, 77	0
All	All	1312/1396 (93%)	0.02	9 (0%) 87 91	35, 46, 59, 77	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	193	TYR	2.7
1	D	262	TYR	2.7
1	B	320	ASP	2.4
1	B	185	LEU	2.4
1	D	320	ASP	2.3
1	B	193	TYR	2.1
1	A	193	TYR	2.1
1	A	3	MET	2.0
1	B	77	VAL	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

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, 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	B-factors(Å ²)	Q<0.9
2	CL	D	417	1/1	0.83	0.08	61,61,61,61	0
2	CL	A	413	1/1	0.89	0.08	60,60,60,60	0
2	CL	B	418	1/1	0.89	0.13	58,58,58,58	0
2	CL	A	411	1/1	0.94	0.17	31,31,31,31	0
2	CL	A	408	1/1	0.96	0.06	40,40,40,40	0
2	CL	C	415	1/1	0.96	0.10	55,55,55,55	0
2	CL	D	421	1/1	0.96	0.23	19,19,19,19	0
2	CL	C	410	1/1	0.97	0.17	30,30,30,30	0
2	CL	D	403	1/1	0.98	0.10	31,31,31,31	0
2	CL	B	412	1/1	0.98	0.18	37,37,37,37	0
2	CL	D	416	1/1	0.98	0.16	37,37,37,37	0
2	CL	B	420	1/1	0.98	0.22	19,19,19,19	0
2	CL	D	401	1/1	0.98	0.16	33,33,33,33	0
2	CL	A	407	1/1	0.99	0.17	28,28,28,28	0
2	CL	A	422	1/1	0.99	0.25	18,18,18,18	0
2	CL	B	402	1/1	0.99	0.20	28,28,28,28	0
2	CL	B	409	1/1	0.99	0.12	39,39,39,39	0
2	CL	C	405	1/1	0.99	0.08	39,39,39,39	0
2	CL	C	404	1/1	0.99	0.09	36,36,36,36	0
2	CL	C	419	1/1	0.99	0.23	17,17,17,17	0
2	CL	C	406	1/1	0.99	0.18	28,28,28,28	0
2	CL	D	414	1/1	0.99	0.06	39,39,39,39	0

6.5 Other polymers

There are no such residues in this entry.