



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:52 AM UTC

PDB ID : 1ZSV / pdb_00001zsv
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 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

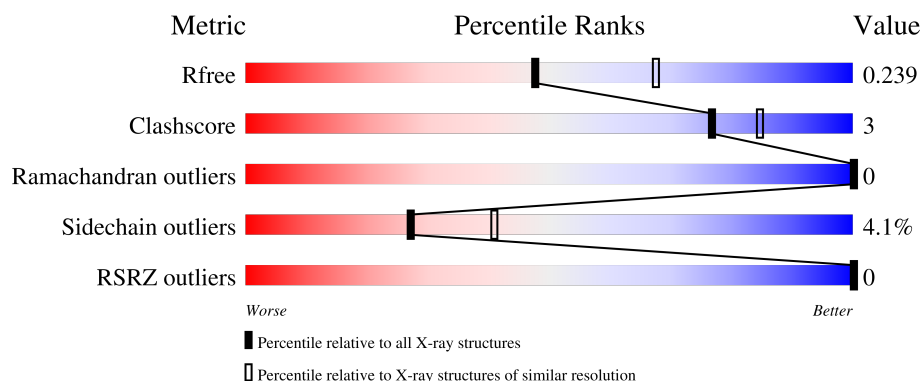
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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 $\leq 5\%$. 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	 83% 9% • 6%
1	B	349	 85% 8% • 6%
1	C	349	 84% 9% • 6%
1	D	349	 85% 9% • 6%

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	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 (CCD ID: CL) (formula: Cl).

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

- Molecule 3 is water.

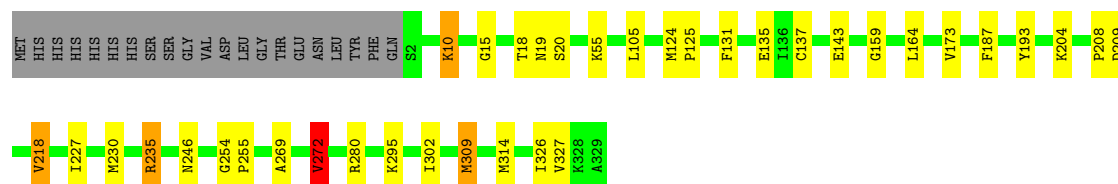
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	84	Total 84	O 84	0	0
3	B	71	Total 71	O 71	0	0
3	C	84	Total 84	O 84	0	0
3	D	76	Total 76	O 76	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

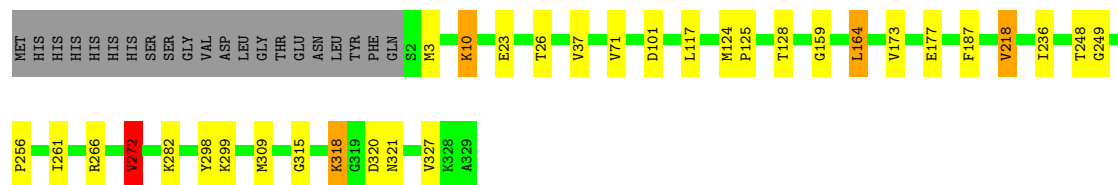
- Molecule 1: NADP-dependent leukotriene B4 12-hydroxydehydrogenase

Chain A: 



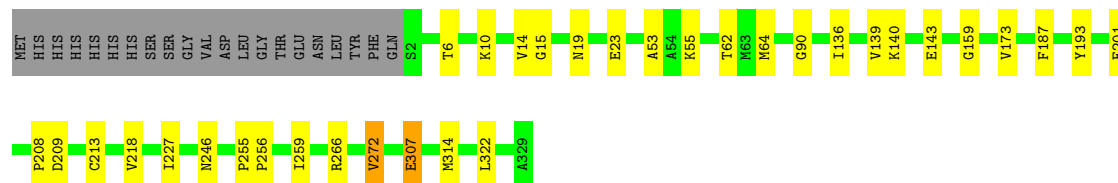
- Molecule 1: NADP-dependent leukotriene B4 12-hydroxydehydrogenase

Chain B: 



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

Chain C: 



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

Chain D: 





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 62.30 – 2.30	Depositor EDS
% Data completeness (in resolution range)	98.4 (62.30-2.30) 98.4 (62.30-2.30)	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 , 0.239	Depositor DCC
R_{free} test set	1917 reflections (2.54%)	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 , 19.2	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	0.96	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	1.03	1/2516 (0.0%)	1.08	7/3409 (0.2%)
1	B	1.02	3/2502 (0.1%)	1.06	5/3398 (0.1%)
1	C	1.02	1/2507 (0.0%)	1.06	5/3399 (0.1%)
1	D	1.02	0/2515	1.05	4/3413 (0.1%)
All	All	1.02	5/10040 (0.0%)	1.06	21/13619 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	218	VAL	CA-CB	6.42	1.62	1.54
1	B	256	PRO	CA-C	5.37	1.57	1.52
1	B	218	VAL	CA-CB	5.08	1.61	1.54
1	B	236	ILE	C-O	-5.04	1.18	1.24
1	C	322	LEU	CA-C	5.02	1.59	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	272	VAL	CB-CA-C	-10.09	98.82	112.04
1	D	272	VAL	CB-CA-C	-8.72	100.61	112.04
1	B	272	VAL	CB-CA-C	-8.32	101.14	112.04
1	B	272	VAL	N-CA-C	7.06	118.67	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	272	VAL	N-CA-C	6.78	118.35	110.62
1	C	208	PRO	CA-C-N	6.68	129.90	120.28
1	C	208	PRO	C-N-CA	6.68	129.90	120.28
1	A	272	VAL	CB-CA-C	-6.39	100.82	111.29
1	D	47	ASP	CA-C-N	6.05	126.22	119.32
1	D	47	ASP	C-N-CA	6.05	126.22	119.32
1	A	208	PRO	CA-C-N	5.95	128.85	120.28
1	A	208	PRO	C-N-CA	5.95	128.85	120.28
1	A	254	GLY	CA-C-N	5.66	126.21	120.38
1	A	254	GLY	C-N-CA	5.66	126.21	120.38
1	A	280	ARG	N-CA-C	5.41	117.17	111.28
1	B	321	ASN	N-CA-C	5.20	117.88	109.40
1	C	272	VAL	N-CA-C	5.17	116.52	110.62
1	B	248	THR	CA-C-N	-5.17	113.76	121.87
1	B	248	THR	C-N-CA	-5.17	113.76	121.87
1	C	272	VAL	N-CA-CB	5.07	116.81	110.47
1	A	235	ARG	NE-CZ-NH2	5.04	123.74	119.20

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 [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	2465	0	2496	15	0
1	B	2450	0	2438	17	0
1	C	2456	0	2479	15	0
1	D	2463	0	2462	13	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	58	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 (58) 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:B:3:MET:HE3	1:B:26:THR:HG22	1.85	0.59
1:C:266:ARG:CD	3:C:447:HOH:O	2.52	0.57
1:B:164:LEU:C	1:B:164:LEU:HD12	2.31	0.56
1:D:193:TYR:CD2	2:D:401:CL:CL	2.96	0.55
1:D:3:MET:HE3	1:D:26:THR:HG22	1.88	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: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:O	1:D:164:LEU:HD12	2.15	0.46
1:B:159:GLY:HA3	1:B:187:PHE:CZ	2.51	0.46
1:C:19:ASN:OD1	1:C:314:MET:HE1	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:GLU:H	1:C:307:GLU:CD	2.23	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:D:49:TYR:C	1:D:49:TYR:CD1	2.94	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:C:53:ALA:HB1	1:C:64:MET:HE2	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
1:A:19:ASN:OD1	1:A:314:MET:HE1	2.20	0.42
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:OD1	1:B:101:ASP:N	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:D:43:PHE:HE1	1:D:328:LYS:HG3	1.86	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 ⓘ

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%)	243 (95%)	13 (5%)	21	32
1	B	250/288 (87%)	243 (97%)	7 (3%)	38	56
1	C	254/288 (88%)	244 (96%)	10 (4%)	28	43
1	D	254/288 (88%)	242 (95%)	12 (5%)	23	35
All	All	1014/1152 (88%)	972 (96%)	42 (4%)	27	41

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LYS
1	A	18	THR
1	A	55	LYS
1	A	105	LEU
1	A	143	GLU
1	A	164	LEU
1	A	173	VAL
1	A	204	LYS
1	A	209	ASP
1	A	218	VAL
1	A	272	VAL
1	A	295	LYS
1	A	309	MET

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Mol	Chain	Res	Type
1	B	10	LYS
1	B	164	LEU
1	B	173	VAL
1	B	218	VAL
1	B	272	VAL
1	B	282	LYS
1	B	318	LYS
1	C	55	LYS
1	C	136	ILE
1	C	140	LYS
1	C	143	GLU
1	C	173	VAL
1	C	201	GLU
1	C	209	ASP
1	C	218	VAL
1	C	272	VAL
1	C	307	GLU
1	D	11	LYS
1	D	34	ASN
1	D	116	SER
1	D	117	LEU
1	D	135	GLU
1	D	147	VAL
1	D	173	VAL
1	D	204	LYS
1	D	218	VAL
1	D	272	VAL
1	D	281	GLN
1	D	304	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	217	ASN
1	B	263	GLN
1	B	281	GLN
1	C	217	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-1.18	0 100 100	35, 46, 59, 70	0
1	B	328/349 (93%)	-1.17	0 100 100	37, 46, 59, 76	0
1	C	328/349 (93%)	-1.19	0 100 100	36, 45, 59, 71	0
1	D	328/349 (93%)	-1.16	0 100 100	35, 46, 59, 77	0
All	All	1312/1396 (93%)	-1.18	0 100 100	35, 46, 59, 77	0

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	A	413	1/1	0.98	0.06	60,60,60,60	0
2	CL	D	417	1/1	0.98	0.05	61,61,61,61	0
2	CL	A	408	1/1	0.99	0.04	40,40,40,40	0
2	CL	B	412	1/1	0.99	0.05	37,37,37,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	B	418	1/1	0.99	0.07	58,58,58,58	0
2	CL	C	410	1/1	0.99	0.04	30,30,30,30	0
2	CL	C	415	1/1	0.99	0.06	55,55,55,55	0
2	CL	D	403	1/1	0.99	0.02	31,31,31,31	0
2	CL	D	416	1/1	0.99	0.05	37,37,37,37	0
2	CL	A	411	1/1	0.99	0.04	31,31,31,31	0
2	CL	D	421	1/1	0.99	0.04	19,19,19,19	0
2	CL	C	405	1/1	1.00	0.02	39,39,39,39	0
2	CL	C	406	1/1	1.00	0.02	28,28,28,28	0
2	CL	B	402	1/1	1.00	0.03	28,28,28,28	0
2	CL	B	409	1/1	1.00	0.02	39,39,39,39	0
2	CL	C	419	1/1	1.00	0.04	17,17,17,17	0
2	CL	D	401	1/1	1.00	0.02	33,33,33,33	0
2	CL	A	407	1/1	1.00	0.01	28,28,28,28	0
2	CL	D	414	1/1	1.00	0.02	39,39,39,39	0
2	CL	A	422	1/1	1.00	0.05	18,18,18,18	0
2	CL	B	420	1/1	1.00	0.04	19,19,19,19	0
2	CL	C	404	1/1	1.00	0.02	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.