



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:06 PM UTC

PDB ID : 3NSQ / pdb_00003nsq
Title : Crystal structure of tetrameric RXRalpha-LBD complexed with antagonist danthron
Authors : Zhang, H.; Hu, T.; Li, L.; Zhou, R.; Chen, L.; Hu, L.; Jiang, H.; Shen, X.
Deposited on : 2010-07-02
Resolution : 2.60 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)	:	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

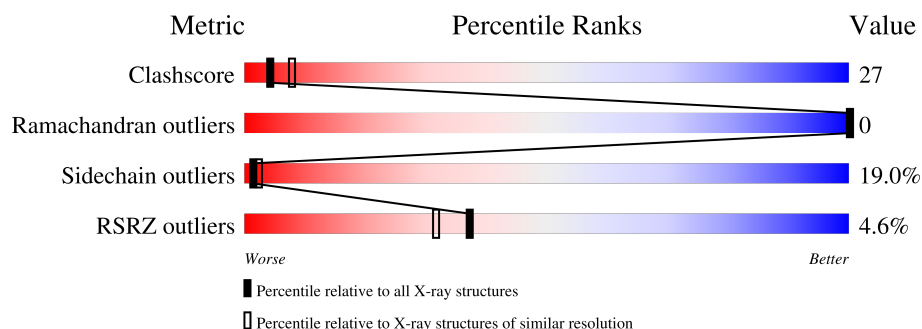
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	240	
1	B	240	

2 Entry composition [i](#)

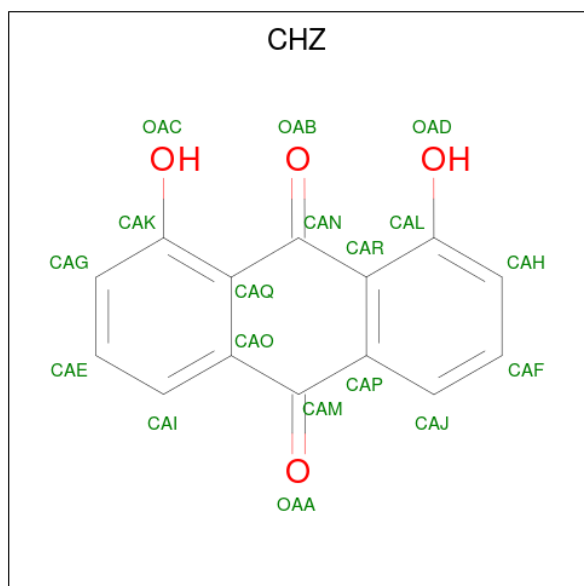
There are 3 unique types of molecules in this entry. The entry contains 3201 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Retinoid X receptor, alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	193	Total	C	N	O	S	0	0	0
			1526	983	264	270	9			
1	B	199	Total	C	N	O	S	0	0	0
			1573	1012	273	278	10			

- Molecule 2 is 1,8-dihydroxyanthracene-9,10-dione (CCD ID: CHZ) (formula: C₁₄H₈O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			18	14	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	46	Total	O	0	0
			46	46		

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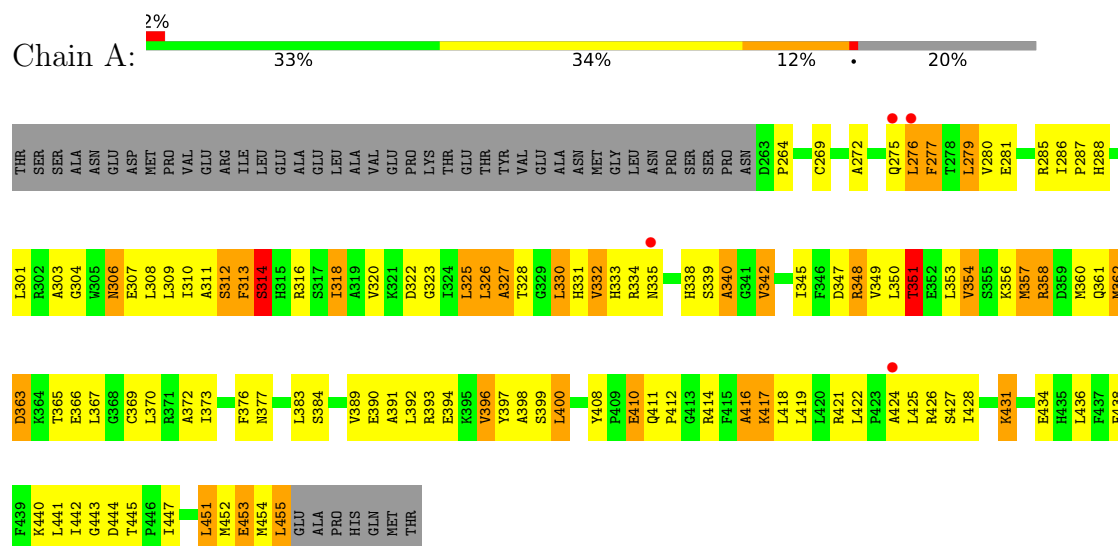
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	38	Total	O	0	0
			38	38		

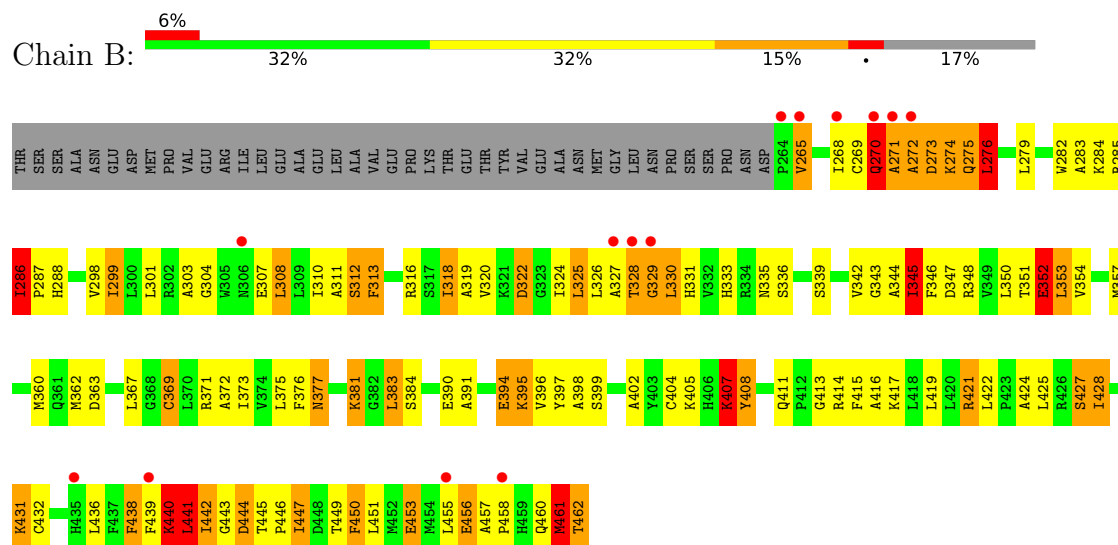
3 Residue-property plots

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: Retinoid X receptor, alpha



• Molecule 1: Retinoid X receptor, alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	115.03Å 99.92Å 47.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.88 – 2.60 14.88 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.4 (14.88-2.60) 94.8 (14.88-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.39 (at 2.61Å)	Xtriage
Refinement program	CNS, REFMAC 5.2.0019	Depositor
R, R_{free}	0.265 , 0.318 0.266 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	43.6	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	3201	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% of the height of the origin peak. No significant pseudotranslation is detected.*

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: CHZ

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	2.23	39/1558 (2.5%)	1.53	21/2106 (1.0%)
1	B	2.25	43/1607 (2.7%)	1.55	26/2172 (1.2%)
All	All	2.24	82/3165 (2.6%)	1.54	47/4278 (1.1%)

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	422	LEU	C-O	-8.43	1.16	1.24
1	A	426	ARG	C-O	-7.79	1.15	1.24
1	B	375	LEU	C-O	-7.44	1.15	1.24
1	B	398	ALA	CA-CB	-7.03	1.42	1.53
1	B	422	LEU	C-O	-7.03	1.18	1.24
1	A	398	ALA	CA-CB	-6.94	1.42	1.53
1	B	445	THR	C-O	-6.78	1.18	1.24
1	A	327	ALA	CA-CB	-6.74	1.44	1.53
1	A	367	LEU	C-O	-6.74	1.16	1.24
1	B	416	ALA	CA-CB	-6.68	1.42	1.53
1	B	271	ALA	CA-CB	-6.65	1.44	1.52
1	B	421	ARG	C-O	-6.31	1.15	1.24
1	B	282	TRP	C-O	-6.27	1.16	1.24
1	B	371	ARG	C-O	-6.27	1.16	1.24
1	B	343	GLY	C-O	-6.20	1.16	1.23
1	B	424	ALA	C-O	-6.17	1.16	1.24
1	B	308	LEU	C-O	-6.17	1.17	1.24
1	A	304	GLY	C-O	-6.16	1.15	1.23
1	A	345	ILE	C-O	-6.04	1.17	1.24
1	B	272	ALA	CA-CB	-6.02	1.44	1.53
1	A	424	ALA	C-O	-5.94	1.17	1.24
1	B	416	ALA	C-O	-5.92	1.17	1.24
1	B	311	ALA	CA-CB	-5.89	1.44	1.53
1	B	347	ASP	C-O	-5.87	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	349	VAL	C-O	-5.85	1.17	1.24
1	A	376	PHE	C-O	-5.84	1.17	1.23
1	A	308	LEU	C-O	-5.83	1.17	1.24
1	A	391	ALA	C-O	-5.81	1.17	1.24
1	A	309	LEU	C-O	-5.80	1.17	1.24
1	B	276	LEU	C-O	-5.80	1.17	1.24
1	B	369	CYS	C-O	-5.80	1.17	1.24
1	A	303	ALA	CA-CB	-5.79	1.43	1.53
1	B	424	ALA	CA-CB	-5.75	1.44	1.53
1	A	438	PHE	C-O	-5.71	1.17	1.24
1	A	417	LYS	C-O	-5.70	1.17	1.24
1	A	389	VAL	C-O	-5.64	1.17	1.24
1	B	377	ASN	C-O	-5.62	1.18	1.24
1	B	372	ALA	C-O	-5.59	1.17	1.24
1	B	298	VAL	C-O	-5.58	1.17	1.24
1	B	413	GLY	C-O	-5.58	1.17	1.24
1	A	314	SER	C-O	-5.57	1.17	1.24
1	A	392	LEU	C-O	-5.55	1.17	1.24
1	A	377	ASN	C-O	-5.54	1.18	1.24
1	B	391	ALA	CA-CB	-5.53	1.44	1.53
1	B	431	LYS	C-O	-5.50	1.17	1.24
1	A	400	LEU	C-O	-5.48	1.17	1.24
1	B	419	LEU	C-O	-5.43	1.17	1.24
1	A	443	GLY	C-O	-5.42	1.16	1.23
1	B	319	ALA	CA-CB	-5.41	1.44	1.53
1	B	299	ILE	C-O	-5.40	1.17	1.24
1	A	340	ALA	CA-CB	-5.36	1.45	1.53
1	A	362	MET	C-O	-5.35	1.17	1.23
1	B	283	ALA	C-O	-5.35	1.17	1.24
1	B	354	VAL	C-O	-5.34	1.18	1.24
1	B	404	CYS	C-O	-5.32	1.17	1.24
1	A	428	ILE	C-O	-5.29	1.18	1.24
1	B	432	CYS	C-O	-5.29	1.17	1.24
1	A	372	ALA	C-O	-5.28	1.18	1.24
1	A	354	VAL	C-O	-5.28	1.18	1.24
1	B	376	PHE	C-O	-5.27	1.18	1.23
1	A	396	VAL	C-O	-5.27	1.18	1.24
1	A	350	LEU	C-O	-5.25	1.17	1.24
1	B	344	ALA	C-O	-5.25	1.18	1.24
1	B	363	ASP	C-O	-5.24	1.17	1.23
1	B	415	PHE	C-O	-5.21	1.18	1.24
1	B	428	ILE	C-O	-5.19	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	353	LEU	C-O	-5.19	1.17	1.23
1	A	279	LEU	C-O	-5.16	1.18	1.24
1	B	310	ILE	C-O	-5.15	1.18	1.24
1	A	441	LEU	CA-C	-5.13	1.47	1.53
1	A	353	LEU	C-O	-5.13	1.17	1.24
1	A	340	ALA	CA-C	-5.13	1.46	1.52
1	B	342	VAL	C-O	-5.10	1.18	1.24
1	A	348	ARG	C-O	-5.09	1.18	1.24
1	A	419	LEU	C-O	-5.09	1.17	1.24
1	B	318	ILE	CA-CB	-5.07	1.46	1.54
1	A	311	ALA	C-O	-5.07	1.18	1.24
1	A	357	MET	CA-C	-5.07	1.46	1.52
1	B	402	ALA	C-O	-5.05	1.18	1.24
1	A	445	THR	C-O	-5.05	1.19	1.24
1	A	416	ALA	C-O	-5.00	1.18	1.24
1	B	405	LYS	C-O	-5.00	1.18	1.24

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	277	PHE	N-CA-C	-15.17	94.44	113.55
1	B	270	GLN	N-CA-C	-11.53	99.18	113.01
1	B	303	ALA	N-CA-C	8.92	121.08	111.36
1	A	328	THR	N-CA-C	-8.80	102.55	113.38
1	A	276	LEU	CB-CA-C	-8.65	93.83	110.35
1	A	312	SER	N-CA-C	8.31	120.11	111.14
1	A	306	ASN	N-CA-C	7.88	119.65	111.14
1	A	340	ALA	N-CA-C	-7.77	102.81	111.28
1	B	352	GLU	N-CA-C	7.75	119.81	111.36
1	B	301	LEU	N-CA-C	7.73	119.78	111.36
1	A	358	ARG	N-CA-C	7.70	119.31	111.07
1	B	351	THR	N-CA-C	7.62	119.37	111.14
1	A	453	GLU	N-CA-C	-7.57	101.19	110.88
1	A	350	LEU	N-CA-C	7.54	119.58	111.36
1	B	440	LYS	N-CA-C	-7.42	95.00	110.80
1	B	265	VAL	N-CA-C	7.26	117.39	110.42
1	A	357	MET	N-CA-C	-7.20	103.43	111.28
1	B	407	LYS	N-CA-C	7.03	119.03	111.36
1	B	399	SER	N-CA-C	6.70	118.66	111.36
1	A	309	LEU	N-CA-C	6.59	118.25	111.14
1	B	285	ARG	N-CA-C	6.20	119.02	111.82
1	B	408	TYR	CA-C-N	6.17	125.73	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	408	TYR	C-N-CA	6.17	125.73	119.19
1	B	461	MET	N-CA-C	6.08	118.72	107.60
1	B	453	GLU	N-CA-C	6.04	118.83	111.82
1	A	441	LEU	N-CA-C	-6.04	103.45	111.96
1	A	314	SER	N-CA-C	6.00	117.90	111.36
1	B	441	LEU	N-CA-C	5.80	119.12	111.28
1	A	326	LEU	N-CA-C	5.80	120.35	113.28
1	A	332	VAL	N-CA-C	5.75	117.63	108.89
1	B	286	ILE	CB-CA-C	-5.68	105.32	110.88
1	B	350	LEU	N-CA-C	5.59	117.18	111.14
1	B	299	ILE	CB-CA-C	-5.58	104.61	112.14
1	B	329	GLY	N-CA-C	-5.55	107.60	115.43
1	B	421	ARG	CA-C-N	5.52	126.63	120.06
1	B	421	ARG	C-N-CA	5.52	126.63	120.06
1	A	354	VAL	N-CA-C	5.42	116.15	110.62
1	B	396	VAL	N-CA-C	5.42	115.62	110.42
1	A	434	GLU	N-CA-C	5.37	117.21	111.36
1	B	438	PHE	N-CA-C	5.28	117.03	111.28
1	A	455	LEU	CA-CB-CG	-5.21	98.08	116.30
1	B	396	VAL	CB-CA-C	-5.17	105.36	111.97
1	B	345	ILE	N-CA-C	5.16	115.93	110.72
1	B	312	SER	N-CA-C	5.15	116.71	111.14
1	A	408	TYR	CB-CA-C	-5.12	104.51	111.21
1	A	396	VAL	CB-CA-C	-5.06	105.50	111.97
1	A	351	THR	N-CA-C	5.03	116.58	111.14

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	1526	0	1567	65	1
1	B	1573	0	1613	107	2
2	B	18	0	6	1	0
3	A	46	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	38	0	0	4	0
All	All	3201	0	3186	171	2

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 27.

All (171) 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:440:LYS:C	1:B:441:LEU:HD12	1.42	1.42
1:B:440:LYS:C	1:B:441:LEU:CD1	1.96	1.37
1:B:440:LYS:O	1:B:441:LEU:CD1	1.84	1.24
1:B:440:LYS:O	1:B:441:LEU:HD13	1.10	1.22
1:B:451:LEU:O	1:B:455:LEU:HD13	1.45	1.17
1:B:441:LEU:HD12	1:B:441:LEU:N	1.59	1.08
1:B:456:GLU:H	1:B:456:GLU:CD	1.57	1.03
1:B:407:LYS:HD2	1:B:408:TYR:CE1	1.95	1.02
1:A:366:GLU:OE2	1:A:414:ARG:NH2	1.92	1.01
1:B:460:GLN:O	1:B:461:MET:HG2	1.59	1.01
1:A:454:MET:O	1:A:454:MET:HG3	1.63	0.96
1:B:447:ILE:O	1:B:451:LEU:HD13	1.63	0.96
1:A:276:LEU:O	1:A:276:LEU:HG	1.70	0.91
1:B:460:GLN:C	1:B:461:MET:HG2	1.92	0.90
1:A:310:ILE:O	1:A:314:SER:OG	1.89	0.90
1:A:275:GLN:O	1:A:276:LEU:CB	2.21	0.89
1:B:440:LYS:HG2	1:B:441:LEU:HD12	1.55	0.88
1:A:366:GLU:CD	1:A:414:ARG:HH21	1.80	0.88
1:B:456:GLU:CD	1:B:456:GLU:N	2.28	0.87
1:A:316:ARG:HG2	1:A:325:LEU:HD23	1.56	0.86
1:B:268:ILE:O	1:B:269:CYS:HB3	1.74	0.86
1:B:369:CYS:O	1:B:373:ILE:HG13	1.76	0.86
1:B:345:ILE:HD12	1:B:345:ILE:O	1.75	0.85
1:A:275:GLN:O	1:A:276:LEU:HB3	1.78	0.82
1:B:327:ALA:O	1:B:328:THR:HG22	1.81	0.81
1:B:442:ILE:O	1:B:446:PRO:HD3	1.81	0.80
1:B:322:ASP:OD1	1:B:333:HIS:ND1	2.16	0.77
1:A:285:ARG:HD2	3:A:73:HOH:O	1.85	0.76
1:A:454:MET:O	1:A:454:MET:CG	2.30	0.75
1:B:451:LEU:O	1:B:455:LEU:CD1	2.31	0.74
1:A:272:ALA:O	1:A:275:GLN:O	2.07	0.72
1:A:326:LEU:O	1:A:327:ALA:HB3	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:LYS:HG3	1:B:275:GLN:N	2.03	0.71
1:B:442:ILE:O	1:B:446:PRO:CD	2.38	0.71
1:B:326:LEU:HD12	1:B:330:LEU:CD1	2.21	0.70
1:A:373:ILE:O	1:A:393:ARG:NH2	2.24	0.69
1:B:326:LEU:HB2	1:B:330:LEU:HD12	1.75	0.68
1:A:369:CYS:HB2	1:A:400:LEU:HD13	1.75	0.68
1:B:462:THR:O	1:B:462:THR:HG22	1.94	0.68
1:B:362:MET:HE3	1:B:367:LEU:HA	1.76	0.67
1:B:328:THR:HG22	1:B:330:LEU:HB2	1.77	0.67
1:A:307:GLU:HG2	1:A:425:LEU:HG	1.76	0.66
1:B:462:THR:O	1:B:462:THR:CG2	2.44	0.65
1:B:318:ILE:O	1:B:318:ILE:HG22	1.96	0.65
1:B:444:ASP:N	1:B:444:ASP:OD1	2.29	0.65
1:B:273:ASP:OD2	1:B:273:ASP:N	2.30	0.64
1:A:390:GLU:O	1:A:394:GLU:HG3	1.97	0.64
1:B:460:GLN:N	1:B:460:GLN:OE1	2.30	0.64
1:B:276:LEU:HD13	1:B:276:LEU:O	1.98	0.63
1:B:440:LYS:HG2	1:B:441:LEU:CD1	2.27	0.63
1:A:314:SER:O	1:A:354:VAL:HG22	1.98	0.63
1:A:373:ILE:CD1	1:A:397:TYR:HB3	2.29	0.62
1:A:318:ILE:O	1:A:358:ARG:NH1	2.32	0.62
1:B:288:HIS:CE1	1:B:395:LYS:HE3	2.34	0.62
1:B:421:ARG:HH11	1:B:421:ARG:HG2	1.64	0.61
1:B:449:THR:O	1:B:453:GLU:HG3	2.01	0.61
1:B:362:MET:HE2	1:B:367:LEU:HB2	1.82	0.61
1:A:363:ASP:C	1:A:363:ASP:OD2	2.43	0.61
1:A:373:ILE:HD11	1:A:397:TYR:HB3	1.81	0.60
1:B:269:CYS:C	1:B:271:ALA:N	2.54	0.60
1:A:347:ASP:O	1:A:351:THR:OG1	2.15	0.60
1:B:348:ARG:O	1:B:352:GLU:HB2	2.01	0.60
1:A:414:ARG:O	1:A:418:LEU:HG	2.02	0.59
1:A:276:LEU:O	1:A:276:LEU:CG	2.44	0.59
1:A:369:CYS:CB	1:A:400:LEU:HD13	2.33	0.58
1:B:439:PHE:C	1:B:440:LYS:O	2.41	0.58
1:B:407:LYS:HD2	1:B:408:TYR:CZ	2.39	0.58
1:B:287:PRO:O	1:B:288:HIS:HB2	2.04	0.57
1:B:460:GLN:O	1:B:461:MET:CG	2.46	0.57
1:A:357:MET:HG2	1:A:362:MET:SD	2.45	0.57
1:A:335:ASN:H	1:A:338:HIS:HD2	1.53	0.57
1:A:320:VAL:HG11	1:A:331:HIS:NE2	2.19	0.57
1:B:443:GLY:O	1:B:447:ILE:HG12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:GLU:O	1:A:453:GLU:HG3	2.04	0.56
1:B:460:GLN:N	1:B:460:GLN:CD	2.62	0.56
1:B:407:LYS:CD	1:B:408:TYR:CE1	2.82	0.56
1:B:446:PRO:O	1:B:450:PHE:HB2	2.05	0.56
1:B:438:PHE:C	1:B:440:LYS:H	2.13	0.56
1:B:268:ILE:CG2	1:B:269:CYS:N	2.69	0.55
1:A:436:LEU:HB2	1:A:440:LYS:HE3	1.87	0.55
1:B:268:ILE:HG22	1:B:269:CYS:N	2.20	0.55
1:B:394:GLU:HG2	1:B:397:TYR:CZ	2.42	0.55
1:B:348:ARG:NH2	1:B:427:SER:OG	2.41	0.54
1:B:360:MET:CE	1:B:417:LYS:HD3	2.38	0.53
1:B:421:ARG:NH1	3:B:22:HOH:O	2.41	0.53
1:B:269:CYS:C	1:B:271:ALA:H	2.19	0.51
1:B:326:LEU:HD22	3:B:35:HOH:O	2.11	0.51
1:B:362:MET:HE3	1:B:367:LEU:CA	2.41	0.51
1:B:421:ARG:HG2	1:B:421:ARG:NH1	2.26	0.51
1:B:456:GLU:N	1:B:456:GLU:OE1	2.30	0.51
1:B:390:GLU:OE1	1:B:390:GLU:O	2.30	0.50
1:A:348:ARG:HH11	1:A:431:LYS:HZ3	1.59	0.50
1:B:327:ALA:O	1:B:330:LEU:CB	2.59	0.50
1:A:275:GLN:O	1:A:276:LEU:HB2	2.08	0.50
1:A:306:ASN:O	1:A:310:ILE:HG13	2.12	0.50
1:B:276:LEU:HD13	1:B:276:LEU:C	2.37	0.49
1:B:326:LEU:HD12	1:B:330:LEU:HD12	1.95	0.49
1:A:366:GLU:OE1	1:A:414:ARG:NE	2.36	0.49
1:B:407:LYS:CD	1:B:408:TYR:CZ	2.96	0.49
1:A:339:SER:O	1:A:340:ALA:C	2.55	0.49
1:A:451:LEU:O	1:A:454:MET:HB3	2.12	0.49
1:B:318:ILE:O	1:B:318:ILE:CG2	2.59	0.48
1:B:394:GLU:HG2	1:B:397:TYR:OH	2.14	0.48
1:A:316:ARG:CZ	1:A:327:ALA:HB2	2.43	0.48
1:A:332:VAL:HG12	1:A:333:HIS:N	2.28	0.48
1:A:306:ASN:O	1:A:310:ILE:HD12	2.13	0.48
1:A:280:VAL:O	1:A:280:VAL:HG12	2.14	0.47
1:A:360:MET:O	1:A:361:GLN:HB2	2.14	0.47
1:A:287:PRO:O	1:A:288:HIS:HB2	2.15	0.47
1:B:438:PHE:O	1:B:440:LYS:N	2.44	0.47
1:B:438:PHE:C	1:B:440:LYS:N	2.72	0.47
1:B:451:LEU:CD1	1:B:451:LEU:N	2.77	0.47
1:B:284:LYS:NZ	3:B:31:HOH:O	2.40	0.47
1:A:348:ARG:HH11	1:A:431:LYS:NZ	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:GLU:HG2	1:A:411:GLN:HG3	1.97	0.47
1:B:270:GLN:C	1:B:272:ALA:H	2.23	0.47
1:A:339:SER:OG	1:A:342:VAL:HG23	2.15	0.46
1:B:270:GLN:HE21	1:B:270:GLN:HB2	1.36	0.46
1:B:451:LEU:N	1:B:451:LEU:HD12	2.30	0.46
1:B:346:PHE:HA	2:B:1:CHZ:HAF	1.97	0.46
1:A:320:VAL:CG1	1:A:331:HIS:NE2	2.79	0.46
1:B:288:HIS:HE1	3:B:61:HOH:O	1.98	0.46
1:B:330:LEU:HD22	1:B:331:HIS:N	2.30	0.46
1:B:362:MET:CE	1:B:367:LEU:HB2	2.45	0.46
1:B:330:LEU:HD22	1:B:330:LEU:C	2.40	0.46
1:B:326:LEU:CD1	1:B:330:LEU:HD12	2.46	0.45
1:B:307:GLU:HG2	1:B:425:LEU:HG	1.97	0.45
1:A:326:LEU:HD12	1:A:330:LEU:HB3	1.98	0.45
1:A:264:PRO:HB2	1:A:447:ILE:HD13	1.98	0.45
1:B:299:ILE:HG21	1:B:383:LEU:HD13	1.99	0.45
1:A:410:GLU:O	1:A:412:PRO:HD3	2.17	0.45
1:A:276:LEU:HA	1:A:279:LEU:HB3	1.97	0.45
1:B:394:GLU:HA	1:B:397:TYR:CE2	2.52	0.45
1:B:304:GLY:O	1:B:308:LEU:HG	2.16	0.44
1:A:360:MET:HE2	1:A:417:LYS:HD3	2.00	0.44
1:A:373:ILE:HD11	1:A:397:TYR:CB	2.47	0.44
1:A:306:ASN:O	1:A:310:ILE:CD1	2.66	0.44
1:B:327:ALA:O	1:B:330:LEU:HB3	2.18	0.44
1:B:286:ILE:N	1:B:286:ILE:HD13	2.33	0.44
1:B:360:MET:HE3	1:B:417:LYS:HD3	2.00	0.43
1:A:370:LEU:HD23	1:A:370:LEU:HA	1.83	0.43
1:A:416:ALA:HB3	1:B:397:TYR:CE1	2.53	0.43
1:B:327:ALA:O	1:B:328:THR:CG2	2.60	0.43
1:B:276:LEU:C	1:B:276:LEU:CD1	2.91	0.43
1:B:273:ASP:HA	1:B:276:LEU:CB	2.49	0.42
1:A:318:ILE:HD13	1:A:318:ILE:HG21	1.80	0.42
1:B:381:LYS:HE3	1:B:381:LYS:HB2	1.78	0.42
1:A:323:GLY:HA3	1:A:331:HIS:NE2	2.33	0.42
1:A:360:MET:CE	1:A:417:LYS:HD3	2.50	0.42
1:A:326:LEU:O	1:A:327:ALA:CB	2.56	0.42
1:B:324:ILE:HD13	1:B:324:ILE:HG21	1.66	0.42
1:A:313:PHE:C	1:A:313:PHE:CD1	2.97	0.42
1:A:342:VAL:HG23	1:A:342:VAL:H	1.62	0.41
1:B:442:ILE:HD12	1:B:442:ILE:HG21	1.80	0.41
1:B:414:ARG:NH1	1:B:414:ARG:HG3	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:LEU:O	1:B:357:MET:HG3	2.20	0.41
1:A:363:ASP:OD2	1:A:365:THR:N	2.54	0.41
1:A:396:VAL:O	1:A:399:SER:OG	2.35	0.41
1:B:268:ILE:O	1:B:269:CYS:CB	2.44	0.41
1:B:377:ASN:OD1	1:B:377:ASN:C	2.64	0.41
1:A:313:PHE:C	1:A:313:PHE:HD1	2.28	0.41
1:B:325:LEU:HD11	1:B:329:GLY:HA2	2.02	0.41
1:B:411:GLN:HE22	1:B:414:ARG:NH1	2.19	0.41
1:B:443:GLY:C	1:B:444:ASP:OD1	2.63	0.41
1:B:326:LEU:CD1	1:B:330:LEU:CD1	2.97	0.40
1:B:313:PHE:CD1	1:B:313:PHE:C	3.00	0.40
1:B:457:ALA:N	1:B:458:PRO:CD	2.84	0.40
1:B:330:LEU:C	1:B:330:LEU:HD13	2.46	0.40
1:B:414:ARG:HG3	1:B:414:ARG:HH11	1.85	0.40
1:A:280:VAL:HG22	1:A:301:LEU:HD13	2.03	0.40
1:B:270:GLN:C	1:B:272:ALA:N	2.78	0.40

All (2) 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)
1:A:269:CYS:SG	1:B:270:GLN:CG[2_655]	1.40	0.80
1:B:335:ASN:ND2	1:B:384:SER:OG[1_556]	1.71	0.49

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	191/240 (80%)	185 (97%)	6 (3%)	0	100	100
1	B	197/240 (82%)	188 (95%)	9 (5%)	0	100	100
All	All	388/480 (81%)	373 (96%)	15 (4%)	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	166/207 (80%)	140 (84%)	26 (16%)	2	4
1	B	171/207 (83%)	133 (78%)	38 (22%)	1	2
All	All	337/414 (81%)	273 (81%)	64 (19%)	1	2

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	PHE
1	A	281	GLU
1	A	286	ILE
1	A	312	SER
1	A	313	PHE
1	A	314	SER
1	A	318	ILE
1	A	322	ASP
1	A	325	LEU
1	A	330	LEU
1	A	334	ARG
1	A	342	VAL
1	A	351	THR
1	A	356	LYS
1	A	363	ASP
1	A	383	LEU
1	A	384	SER
1	A	410	GLU
1	A	421	ARG
1	A	427	SER
1	A	431	LYS
1	A	442	ILE
1	A	444	ASP
1	A	451	LEU
1	A	452	MET

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Mol	Chain	Res	Type
1	A	455	LEU
1	B	265	VAL
1	B	270	GLN
1	B	273	ASP
1	B	274	LYS
1	B	275	GLN
1	B	276	LEU
1	B	279	LEU
1	B	286	ILE
1	B	312	SER
1	B	313	PHE
1	B	316	ARG
1	B	320	VAL
1	B	322	ASP
1	B	325	LEU
1	B	328	THR
1	B	330	LEU
1	B	336	SER
1	B	339	SER
1	B	345	ILE
1	B	352	GLU
1	B	381	LYS
1	B	383	LEU
1	B	394	GLU
1	B	395	LYS
1	B	407	LYS
1	B	427	SER
1	B	428	ILE
1	B	431	LYS
1	B	436	LEU
1	B	440	LYS
1	B	441	LEU
1	B	442	ILE
1	B	444	ASP
1	B	447	ILE
1	B	450	PHE
1	B	456	GLU
1	B	461	MET
1	B	462	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	275	GLN
1	A	288	HIS
1	A	306	ASN
1	A	338	HIS
1	A	411	GLN
1	B	270	GLN
1	B	288	HIS
1	B	411	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](#)

1 ligand is 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	CHZ	B	1	-	20,20,20	1.93	4 (20%)	30,30,30	0.70	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CHZ	B	1	-	-	-	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	CHZ	CAP-CAM	-4.57	1.39	1.48
2	B	1	CHZ	CAO-CAM	-4.46	1.39	1.48
2	B	1	CHZ	CAQ-CAN	-3.52	1.39	1.47
2	B	1	CHZ	CAR-CAN	-3.52	1.39	1.47

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	B	1	CHZ	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	193/240 (80%)	0.48	4 (2%) 63 58	21, 38, 59, 64	0
1	B	199/240 (82%)	0.68	14 (7%) 22 18	20, 37, 64, 71	0
All	All	392/480 (81%)	0.58	18 (4%) 37 32	20, 38, 60, 71	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	271	ALA	4.8
1	B	329	GLY	4.6
1	B	327	ALA	4.4
1	B	264	PRO	3.4
1	B	272	ALA	3.4
1	B	270	GLN	3.4
1	B	439	PHE	3.2
1	B	265	VAL	3.1
1	B	328	THR	3.1
1	A	424	ALA	2.7
1	A	335	ASN	2.5
1	B	455	LEU	2.3
1	B	268	ILE	2.3
1	B	306	ASN	2.3
1	A	275	GLN	2.3
1	A	276	LEU	2.3
1	B	435	HIS	2.2
1	B	458	PRO	2.1

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($\text{\AA}^2$)	Q<0.9
2	CHZ	B	1	18/18	0.70	0.30	72,72,73,73	18

6.5 Other polymers [i](#)

There are no such residues in this entry.