



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:46 AM UTC

PDB ID : 5XR2 / pdb_00005xr2
Title : SAV0551
Authors : Kim, H.J.; Kwon, A.R.; Lee, B.J.
Deposited on : 2017-06-07
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

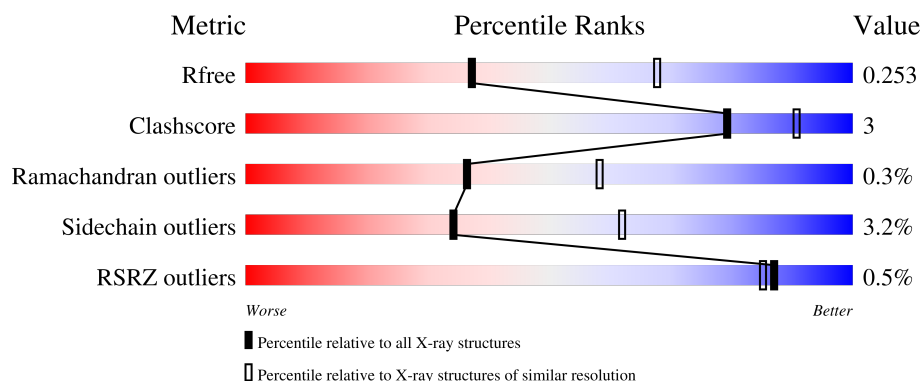
1 Overall quality at a glance

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))
R_{free}	180053	4008 (2.60-2.60)
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	300	% 88% 6% . .
1	B	300	% 84% 11% . 5%
1	C	300	% 85% 12% . .
1	D	300	82% 11% . 5%
1	E	300	88% 7% .

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Mol	Chain	Length	Quality of chain
1	F	300	 83% 11% 6%
1	G	300	 92% 6% ..
1	H	300	 92% ..

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	LAC	A	401	-	X	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18184 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Protein/nucleic acid deglycase HchA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2224	1418	365	432	9			
1	B	286	Total	C	N	O	S	0	0	0
			2214	1411	363	431	9			
1	C	295	Total	C	N	O	S	0	0	0
			2301	1463	386	443	9			
1	D	284	Total	C	N	O	S	0	0	0
			2198	1401	360	428	9			
1	E	287	Total	C	N	O	S	0	0	0
			2224	1416	366	433	9			
1	F	283	Total	C	N	O	S	0	0	0
			2190	1397	359	425	9			
1	G	295	Total	C	N	O	S	0	0	0
			2301	1463	386	443	9			
1	H	289	Total	C	N	O	S	0	0	0
			2239	1424	368	438	9			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	293	LEU	-	expression tag	UNP P64312
A	294	GLU	-	expression tag	UNP P64312
A	295	HIS	-	expression tag	UNP P64312
A	296	HIS	-	expression tag	UNP P64312
A	297	HIS	-	expression tag	UNP P64312
A	298	HIS	-	expression tag	UNP P64312
A	299	HIS	-	expression tag	UNP P64312
A	300	HIS	-	expression tag	UNP P64312
B	293	LEU	-	expression tag	UNP P64312
B	294	GLU	-	expression tag	UNP P64312
B	295	HIS	-	expression tag	UNP P64312
B	296	HIS	-	expression tag	UNP P64312
B	297	HIS	-	expression tag	UNP P64312

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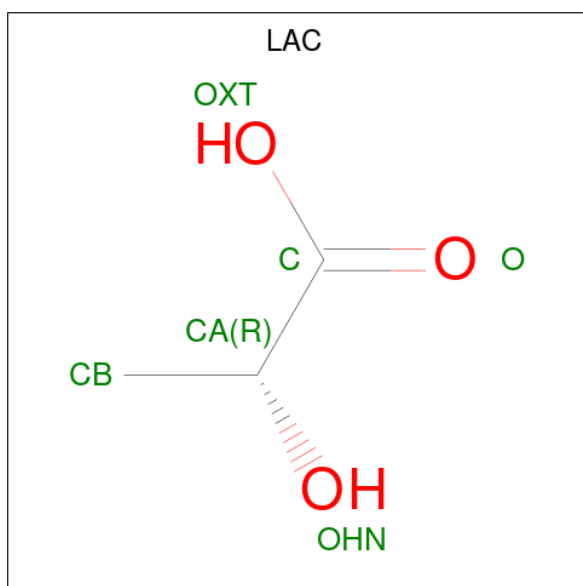
Chain	Residue	Modelled	Actual	Comment	Reference
B	298	HIS	-	expression tag	UNP P64312
B	299	HIS	-	expression tag	UNP P64312
B	300	HIS	-	expression tag	UNP P64312
C	293	LEU	-	expression tag	UNP P64312
C	294	GLU	-	expression tag	UNP P64312
C	295	HIS	-	expression tag	UNP P64312
C	296	HIS	-	expression tag	UNP P64312
C	297	HIS	-	expression tag	UNP P64312
C	298	HIS	-	expression tag	UNP P64312
C	299	HIS	-	expression tag	UNP P64312
C	300	HIS	-	expression tag	UNP P64312
D	293	LEU	-	expression tag	UNP P64312
D	294	GLU	-	expression tag	UNP P64312
D	295	HIS	-	expression tag	UNP P64312
D	296	HIS	-	expression tag	UNP P64312
D	297	HIS	-	expression tag	UNP P64312
D	298	HIS	-	expression tag	UNP P64312
D	299	HIS	-	expression tag	UNP P64312
D	300	HIS	-	expression tag	UNP P64312
E	293	LEU	-	expression tag	UNP P64312
E	294	GLU	-	expression tag	UNP P64312
E	295	HIS	-	expression tag	UNP P64312
E	296	HIS	-	expression tag	UNP P64312
E	297	HIS	-	expression tag	UNP P64312
E	298	HIS	-	expression tag	UNP P64312
E	299	HIS	-	expression tag	UNP P64312
E	300	HIS	-	expression tag	UNP P64312
F	293	LEU	-	expression tag	UNP P64312
F	294	GLU	-	expression tag	UNP P64312
F	295	HIS	-	expression tag	UNP P64312
F	296	HIS	-	expression tag	UNP P64312
F	297	HIS	-	expression tag	UNP P64312
F	298	HIS	-	expression tag	UNP P64312
F	299	HIS	-	expression tag	UNP P64312
F	300	HIS	-	expression tag	UNP P64312
G	293	LEU	-	expression tag	UNP P64312
G	294	GLU	-	expression tag	UNP P64312
G	295	HIS	-	expression tag	UNP P64312
G	296	HIS	-	expression tag	UNP P64312
G	297	HIS	-	expression tag	UNP P64312
G	298	HIS	-	expression tag	UNP P64312
G	299	HIS	-	expression tag	UNP P64312

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Chain	Residue	Modelled	Actual	Comment	Reference
G	300	HIS	-	expression tag	UNP P64312
H	293	LEU	-	expression tag	UNP P64312
H	294	GLU	-	expression tag	UNP P64312
H	295	HIS	-	expression tag	UNP P64312
H	296	HIS	-	expression tag	UNP P64312
H	297	HIS	-	expression tag	UNP P64312
H	298	HIS	-	expression tag	UNP P64312
H	299	HIS	-	expression tag	UNP P64312
H	300	HIS	-	expression tag	UNP P64312

- Molecule 2 is LACTIC ACID (CCD ID: LAC) (formula: $C_3H_6O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 6 3 3	0	0
2	E	1	Total C O 6 3 3	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

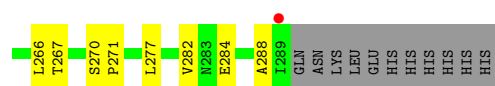
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total Zn 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	64	Total 64	O 64	0	0
4	B	21	Total 21	O 21	0	0
4	C	55	Total 55	O 55	0	0
4	D	21	Total 21	O 21	0	0
4	E	30	Total 30	O 30	0	0
4	F	17	Total 17	O 17	0	0
4	G	50	Total 50	O 50	0	0
4	H	22	Total 22	O 22	0	0

- Molecule 1: Protein/nucleic acid deglycase HchA

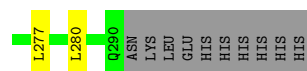
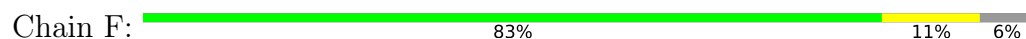




- Molecule 1: Protein/nucleic acid deglycase HchA



- Molecule 1: Protein/nucleic acid deglycase HchA



- Molecule 1: Protein/nucleic acid deglycase HchA



- Molecule 1: Protein/nucleic acid deglycase HchA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.28Å 129.45Å 187.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.65 – 2.60 48.65 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (48.65-2.60) 98.9 (48.65-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.67 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.181 , 0.254 0.187 , 0.253	Depositor DCC
R_{free} test set	3580 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	39.4	Xtrriage
Anisotropy	0.053	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 30.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	18184	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 29.55 % 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 1.5202e-03. 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: ZN, LAC

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	0.96	0/2271	1.02	2/3081 (0.1%)
1	B	0.85	0/2261	0.99	2/3069 (0.1%)
1	C	0.98	4/2354 (0.2%)	1.04	9/3194 (0.3%)
1	D	0.86	1/2245 (0.0%)	0.96	3/3047 (0.1%)
1	E	0.91	0/2271	1.01	0/3081
1	F	0.85	0/2237	0.95	3/3036 (0.1%)
1	G	0.91	0/2354	0.99	3/3194 (0.1%)
1	H	0.83	0/2286	0.95	2/3103 (0.1%)
All	All	0.90	5/18279 (0.0%)	0.99	24/24805 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	189	LEU	C-O	-5.73	1.17	1.23
1	D	228	ILE	CA-C	5.66	1.58	1.52
1	C	145	LEU	N-CA	5.60	1.49	1.46
1	C	297	HIS	CA-C	5.57	1.55	1.52
1	C	158	GLY	C-O	-5.54	1.18	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	251	VAL	N-CA-C	7.98	118.08	110.42
1	C	159	GLY	N-CA-C	-7.88	101.62	112.18
1	F	159	GLY	N-CA-C	-6.74	104.32	112.48
1	C	145	LEU	N-CA-C	6.67	114.25	108.78
1	B	159	GLY	N-CA-C	-6.59	104.51	112.48
1	C	267	THR	CA-C-N	6.45	126.57	121.61
1	C	267	THR	C-N-CA	6.45	126.57	121.61
1	D	159	GLY	N-CA-C	-6.41	103.59	112.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	189	LEU	N-CA-C	6.34	118.71	109.07
1	C	191	HIS	CA-C-N	6.03	125.53	121.13
1	C	191	HIS	C-N-CA	6.03	125.53	121.13
1	A	159	GLY	N-CA-C	-5.82	105.44	112.48
1	H	159	GLY	N-CA-C	-5.79	104.42	112.18
1	F	192	GLY	O-C-N	5.79	123.15	121.07
1	G	274	SER	N-CA-C	5.55	117.01	111.07
1	D	284	GLU	N-CA-C	5.46	117.23	111.28
1	C	190	CYS	CB-CA-C	-5.36	109.95	117.23
1	C	269	ASP	N-CA-C	5.31	119.82	113.23
1	H	189	LEU	N-CA-C	5.24	117.04	108.76
1	C	189	LEU	N-CA-C	5.22	116.78	108.79
1	B	191	HIS	N-CA-C	-5.21	106.93	113.28
1	G	269	ASP	N-CA-C	5.10	119.22	112.89
1	A	37	THR	N-CA-C	-5.09	102.93	110.46
1	F	211	TYR	N-CA-C	-5.08	102.55	110.42

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	2224	0	2221	12	0
1	B	2214	0	2206	15	0
1	C	2301	0	2275	18	0
1	D	2198	0	2189	19	0
1	E	2224	0	2216	10	0
1	F	2190	0	2185	11	0
1	G	2301	0	2275	7	0
1	H	2239	0	2224	4	0
2	A	6	0	0	0	0
2	E	6	0	0	0	0
3	C	1	0	0	0	0
4	A	64	0	0	0	0
4	B	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	55	0	0	0	0
4	D	21	0	0	0	0
4	E	30	0	0	0	0
4	F	17	0	0	0	0
4	G	50	0	0	1	0
4	H	22	0	0	0	0
All	All	18184	0	17791	96	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 (96) 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:A:190:CYS:O	1:A:193:PRO:HD2	1.80	0.81
1:C:270:SER:HB2	1:C:271:PRO:HD2	1.69	0.72
1:G:75:THR:HG21	1:G:160:HIS:HB2	1.70	0.72
1:C:270:SER:HB2	1:C:271:PRO:CD	2.20	0.71
1:C:190:CYS:SG	1:C:191:HIS:N	2.64	0.71
1:B:158:GLY:HA3	1:B:190:CYS:HB3	1.74	0.68
1:C:220:LEU:HD13	1:C:255:MET:HE2	1.83	0.60
1:F:189:LEU:HD22	1:F:277:LEU:HD23	1.86	0.57
1:E:86:LEU:HB3	1:E:90:MET:HE2	1.86	0.57
1:D:218:ASP:OD1	1:D:240:ALA:HB3	2.05	0.56
1:D:53:TRP:CE3	1:D:152:LEU:HD23	2.41	0.56
1:C:220:LEU:CD1	1:C:255:MET:HE2	2.37	0.55
1:F:179:ALA:HB1	1:F:186:ILE:HD11	1.88	0.55
1:A:32:TYR:CZ	1:A:228:ILE:HD11	2.41	0.55
1:D:213:VAL:HG12	1:D:267:THR:HG21	1.89	0.54
1:A:190:CYS:SG	1:A:191:HIS:N	2.81	0.54
1:A:75:THR:OG1	1:A:76:GLY:N	2.41	0.53
1:A:32:TYR:CE2	1:A:228:ILE:HD11	2.43	0.53
1:A:37:THR:HG21	1:A:84:LEU:HD22	1.90	0.53
1:A:39:PHE:HB2	1:A:84:LEU:HD11	1.90	0.53
1:F:179:ALA:CB	1:F:186:ILE:HD11	2.39	0.52
1:E:160:HIS:O	1:E:163:VAL:HG22	2.10	0.51
1:D:244:THR:HG23	1:D:250:VAL:CG2	2.41	0.50
1:D:189:LEU:HD22	1:D:277:LEU:CD2	2.41	0.50
1:A:28:SER:HA	1:A:228:ILE:HD12	1.93	0.50
1:E:188:THR:O	1:E:267:THR:HA	2.12	0.50
1:A:156:ILE:HD12	1:A:156:ILE:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:LEU:HB3	1:B:85:PRO:HD3	1.95	0.49
1:B:153:SER:HB3	1:B:185:PHE:HB2	1.95	0.49
1:C:62:GLU:HG2	1:C:164:VAL:HG11	1.95	0.49
1:F:75:THR:OG1	1:F:109:GLU:OE2	2.31	0.48
1:D:244:THR:HG23	1:D:250:VAL:HG23	1.95	0.48
1:E:58:ILE:HD11	1:E:175:THR:HG21	1.94	0.48
1:G:180:LEU:O	4:G:401:HOH:O	2.20	0.47
1:A:255:MET:HE3	1:A:270:SER:HB2	1.97	0.47
1:E:162:ALA:HB1	1:E:166:ILE:HD11	1.96	0.47
1:H:82:MET:HE1	1:H:106:VAL:HG11	1.97	0.47
1:C:178:TRP:CD1	1:C:182:ASN:HD22	2.33	0.46
1:D:270:SER:HB2	1:D:271:PRO:HD2	1.98	0.46
1:D:156:ILE:HB	1:D:188:THR:HG23	1.97	0.46
1:E:90:MET:HE1	1:E:123:THR:HG23	1.96	0.46
1:C:73:PHE:CE2	1:C:75:THR:HB	2.50	0.46
1:G:189:LEU:N	1:G:189:LEU:HD23	2.31	0.46
1:B:81:GLU:CD	1:B:190:CYS:HB2	2.41	0.46
1:C:190:CYS:O	1:C:193:PRO:HD2	2.16	0.45
1:D:89:LEU:HD23	1:D:282:VAL:HG22	1.97	0.45
1:F:86:LEU:HD13	1:F:127:LEU:HD11	1.97	0.45
1:E:75:THR:OG1	1:E:76:GLY:N	2.48	0.45
1:F:217:PRO:HG2	1:F:220:LEU:HD12	1.97	0.45
1:B:153:SER:CB	1:B:185:PHE:HB2	2.47	0.45
1:D:32:TYR:CE2	1:D:228:ILE:HD11	2.52	0.45
1:D:215:VAL:CG2	1:D:240:ALA:HB2	2.47	0.44
1:B:73:PHE:CE2	1:B:75:THR:HB	2.52	0.44
1:D:189:LEU:HD23	1:D:189:LEU:N	2.33	0.44
1:D:156:ILE:HD13	1:D:195:ALA:CB	2.47	0.44
1:C:81:GLU:OE2	1:C:190:CYS:HB2	2.18	0.44
1:C:9:SER:OG	1:C:11:GLN:HB2	2.18	0.43
1:D:53:TRP:CD2	1:D:152:LEU:HD23	2.53	0.43
1:D:84:LEU:HB3	1:D:85:PRO:HD3	2.00	0.43
1:D:32:TYR:HE2	1:D:228:ILE:HD11	1.82	0.43
1:A:101:LEU:O	1:A:136:LYS:NZ	2.41	0.43
1:F:270:SER:HB2	1:F:271:PRO:HD2	2.01	0.43
1:D:86:LEU:HD21	1:D:155:PHE:CD2	2.54	0.43
1:B:32:TYR:CZ	1:B:228:ILE:HD11	2.54	0.42
1:H:141:ILE:HD11	1:H:171:ASP:O	2.19	0.42
1:B:189:LEU:HD22	1:B:277:LEU:CD2	2.49	0.42
1:F:206:SER:C	1:F:208:LEU:H	2.27	0.42
1:A:151:TYR:O	1:A:184:ARG:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:237:TRP:CE3	1:C:242:LEU:HD22	2.54	0.42
1:G:176:LEU:HD22	1:G:186:ILE:HD13	2.02	0.42
1:B:156:ILE:HD13	1:B:195:ALA:CB	2.49	0.42
1:C:213:VAL:HG12	1:C:267:THR:HG21	2.01	0.42
1:B:213:VAL:CG1	1:B:265:LEU:HD21	2.50	0.42
1:B:32:TYR:CE2	1:B:228:ILE:HD11	2.54	0.42
1:B:188:THR:HG23	1:B:267:THR:HG22	2.02	0.42
1:E:190:CYS:SG	1:E:191:HIS:N	2.92	0.42
1:B:81:GLU:OE1	1:B:190:CYS:HB2	2.20	0.42
1:H:84:LEU:HD12	1:H:84:LEU:HA	1.81	0.42
1:H:189:LEU:N	1:H:189:LEU:HD23	2.35	0.42
1:F:192:GLY:N	1:F:193:PRO:CD	2.83	0.41
1:G:190:CYS:SG	1:G:191:HIS:N	2.93	0.41
1:C:80:VAL:HG22	1:C:114:PRO:HG3	2.02	0.41
1:B:251:VAL:HG11	1:B:260:LEU:HD22	2.01	0.41
1:C:87:HIS:HD1	1:C:123:THR:HG1	1.64	0.41
1:C:153:SER:OG	1:C:185:PHE:HB2	2.21	0.41
1:D:208:LEU:O	1:D:248:LEU:HD22	2.20	0.41
1:E:36:LYS:HA	1:E:117:ASP:HB2	2.02	0.41
1:G:138:ALA:HA	1:G:141:ILE:HD12	2.03	0.41
1:F:32:TYR:CE2	1:F:228:ILE:HD11	2.56	0.41
1:C:84:LEU:HB3	1:C:85:PRO:HD3	2.03	0.41
1:F:84:LEU:HB3	1:F:85:PRO:HD3	2.03	0.41
1:C:178:TRP:CD1	1:C:182:ASN:ND2	2.90	0.40
1:E:213:VAL:HG12	1:E:267:THR:HG21	2.03	0.40
1:D:215:VAL:HG23	1:D:240:ALA:HB2	2.03	0.40
1:B:48:TYR:OH	1:B:50:ASP:HB2	2.21	0.40
1:G:82:MET:HE1	1:G:106:VAL:HG11	2.04	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	285/300 (95%)	265 (93%)	20 (7%)	0	100	100
1	B	284/300 (95%)	266 (94%)	17 (6%)	1 (0%)	30	51
1	C	293/300 (98%)	278 (95%)	15 (5%)	0	100	100
1	D	282/300 (94%)	260 (92%)	20 (7%)	2 (1%)	18	38
1	E	285/300 (95%)	272 (95%)	12 (4%)	1 (0%)	30	51
1	F	281/300 (94%)	265 (94%)	14 (5%)	2 (1%)	18	38
1	G	293/300 (98%)	279 (95%)	14 (5%)	0	100	100
1	H	287/300 (96%)	274 (96%)	12 (4%)	1 (0%)	36	58
All	All	2290/2400 (95%)	2159 (94%)	124 (5%)	7 (0%)	36	58

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	190	CYS
1	B	45	LYS
1	D	288	ALA
1	H	190	CYS
1	D	260	LEU
1	E	190	CYS
1	F	207	PRO

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	244/257 (95%)	239 (98%)	5 (2%)	48	74
1	B	243/257 (95%)	231 (95%)	12 (5%)	22	47
1	C	252/257 (98%)	245 (97%)	7 (3%)	38	66
1	D	241/257 (94%)	229 (95%)	12 (5%)	22	46
1	E	244/257 (95%)	239 (98%)	5 (2%)	48	74
1	F	240/257 (93%)	231 (96%)	9 (4%)	29	56
1	G	252/257 (98%)	246 (98%)	6 (2%)	43	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	H	246/257 (96%)	239 (97%)	7 (3%)	38 66
All	All	1962/2056 (95%)	1899 (97%)	63 (3%)	34 62

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	GLU
1	A	75	THR
1	A	156	ILE
1	A	163	VAL
1	A	251	VAL
1	B	5	VAL
1	B	40	ASP
1	B	84	LEU
1	B	126	LYS
1	B	129	GLU
1	B	136	LYS
1	B	188	THR
1	B	196	LEU
1	B	227	GLU
1	B	251	VAL
1	B	266	LEU
1	B	280	LEU
1	C	11	GLN
1	C	16	LYS
1	C	102	SER
1	C	115	THR
1	C	183	ASP
1	C	201	LEU
1	C	251	VAL
1	D	30	SER
1	D	55	VAL
1	D	131	LEU
1	D	135	LYS
1	D	152	LEU
1	D	153	SER
1	D	167	SER
1	D	188	THR
1	D	189	LEU
1	D	214	CYS
1	D	248	LEU
1	D	266	LEU

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Mol	Chain	Res	Type
1	E	6	ASN
1	E	8	LEU
1	E	49	LYS
1	E	65	VAL
1	E	227	GLU
1	F	49	LYS
1	F	128	LYS
1	F	135	LYS
1	F	163	VAL
1	F	169	SER
1	F	205	LYS
1	F	214	CYS
1	F	219	SER
1	F	280	LEU
1	G	72	MET
1	G	75	THR
1	G	107	LYS
1	G	154	VAL
1	G	163	VAL
1	G	277	LEU
1	H	4	ASP
1	H	9	SER
1	H	84	LEU
1	H	226	ILE
1	H	267	THR
1	H	289	ILE
1	H	291	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	78	HIS
1	B	31	GLN
1	C	6	ASN
1	D	182	ASN
1	E	202	ASN
1	G	20	ASN
1	G	298	HIS
1	G	300	HIS
1	H	6	ASN
1	H	20	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 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	LAC	A	401	-	4,5,5	1.38	1 (25%)	2,6,6	1.96	1 (50%)
2	LAC	E	401	-	4,5,5	0.90	0	2,6,6	0.22	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LAC	A	401	-	-	4/4/4/4	-
2	LAC	E	401	-	-	4/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	LAC	O-C	2.31	1.28	1.22

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	LAC	OXT-C-O	2.46	129.67	124.08

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	LAC	O-C-CA-CB
2	A	401	LAC	O-C-CA-OHN
2	A	401	LAC	OXT-C-CA-CB
2	A	401	LAC	OXT-C-CA-OHN
2	E	401	LAC	O-C-CA-CB
2	E	401	LAC	OXT-C-CA-CB
2	E	401	LAC	OXT-C-CA-OHN
2	E	401	LAC	O-C-CA-OHN

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	287/300 (95%)	-0.64	2 (0%) 84 82	16, 30, 46, 81	0
1	B	286/300 (95%)	-0.20	2 (0%) 84 82	22, 46, 64, 81	0
1	C	295/300 (98%)	-0.53	2 (0%) 84 82	18, 32, 52, 90	0
1	D	284/300 (94%)	-0.11	1 (0%) 88 86	28, 48, 70, 84	0
1	E	287/300 (95%)	-0.38	1 (0%) 90 88	21, 38, 62, 83	0
1	F	283/300 (94%)	-0.14	1 (0%) 88 86	23, 48, 70, 87	0
1	G	295/300 (98%)	-0.58	0 100 100	19, 32, 49, 86	0
1	H	289/300 (96%)	-0.21	2 (0%) 84 82	23, 47, 72, 96	0
All	All	2306/2400 (96%)	-0.35	11 (0%) 87 85	16, 39, 65, 96	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	5	VAL	3.7
1	C	190	CYS	3.7
1	B	5	VAL	3.5
1	F	8	LEU	3.0
1	D	289	ILE	2.8
1	A	190	CYS	2.8
1	H	288	ALA	2.5
1	A	293	LEU	2.2
1	C	300	HIS	2.1
1	E	6	ASN	2.1
1	B	183	ASP	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 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	LAC	E	401	6/6	0.82	0.13	34,36,37,38	0
2	LAC	A	401	6/6	0.85	0.11	30,35,37,37	0
3	ZN	C	401	1/1	0.97	0.03	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.