



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:26 PM GMT

PDB ID : 1TOG
Title : Hydrocinnamic acid-bound structure of SRHEPT + A293D mutant of E. coli aspartate aminotransferase
Authors : Chow, M.A.; McElroy, K.E.; Corbett, K.D.; Berger, J.M.; Kirsch, J.F.
Deposited on : 2004-06-14
Resolution : 2.31 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
<http://wwpdb.org/validation/2016/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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

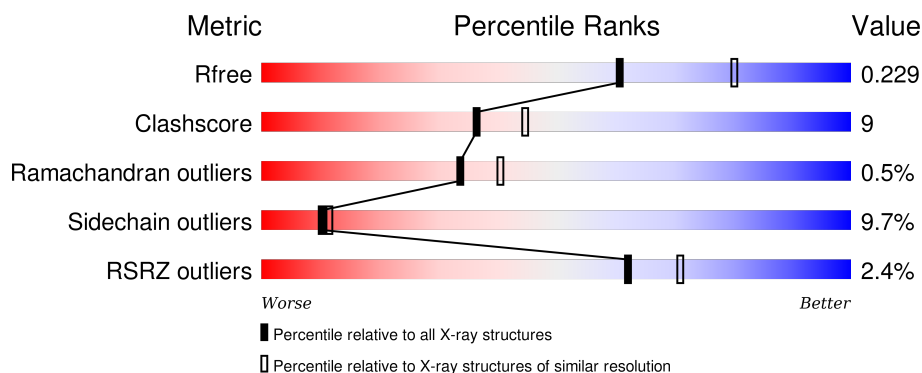
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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}	91344	4425 (2.34-2.30)
Clashscore	102246	5057 (2.34-2.30)
Ramachandran outliers	100387	5008 (2.34-2.30)
Sidechain outliers	100360	5007 (2.34-2.30)
RSRZ outliers	91569	4432 (2.34-2.30)

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. 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	396	<div> <div>3%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
1	B	396	<div> <div>2%</div> <div>75%</div> <div>21%</div> <div>..</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6329 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.

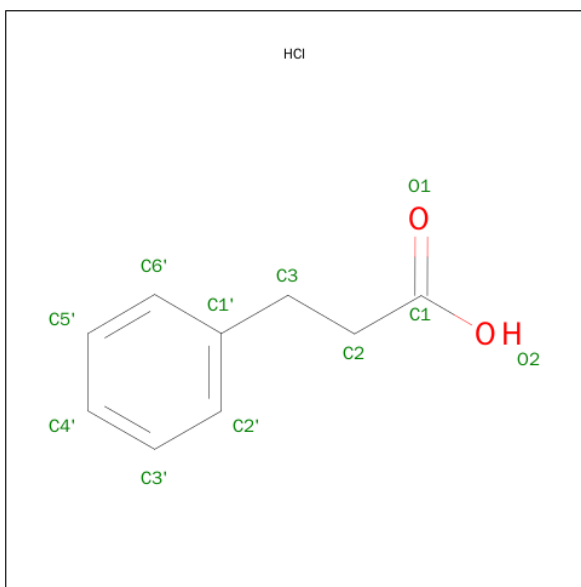
- Molecule 1 is a protein called Aspartate aminotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	P	S	0	0	0
			3085	1943	535	593	1	13			
1	B	396	Total	C	N	O	P	S	0	0	0
			3085	1943	535	593	1	13			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	THR	ALA	ENGINEERED	UNP P00509
A	13	THR	PRO	ENGINEERED	UNP P00509
A	34	ASP	ASN	ENGINEERED	UNP P00509
A	109	SER	THR	ENGINEERED	UNP P00509
A	258	LLP	LYS	MODIFIED RESIDUE	UNP P00509
A	261	ALA	GLY	ENGINEERED	UNP P00509
A	285	GLY	SER	ENGINEERED	UNP P00509
A	293	ASP	ALA	ENGINEERED	UNP P00509
A	297	SER	ASN	ENGINEERED	UNP P00509
B	12	THR	ALA	ENGINEERED	UNP P00509
B	13	THR	PRO	ENGINEERED	UNP P00509
B	34	ASP	ASN	ENGINEERED	UNP P00509
B	109	SER	THR	ENGINEERED	UNP P00509
B	258	LLP	LYS	MODIFIED RESIDUE	UNP P00509
B	261	ALA	GLY	ENGINEERED	UNP P00509
B	285	GLY	SER	ENGINEERED	UNP P00509
B	293	ASP	ALA	ENGINEERED	UNP P00509
B	297	SER	ASN	ENGINEERED	UNP P00509

- Molecule 2 is HYDROCINNAMIC ACID (three-letter code: HCI) (formula: C₉H₁₀O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			11	9	2		
2	B	1	Total	C	O	0	0
			11	9	2		

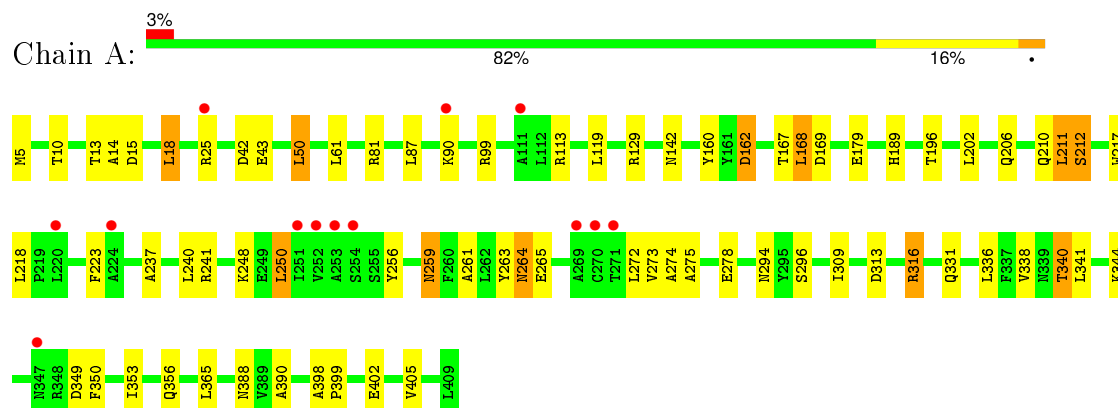
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	60	Total	O	0	0
			60	60		
3	B	77	Total	O	0	0
			77	77		

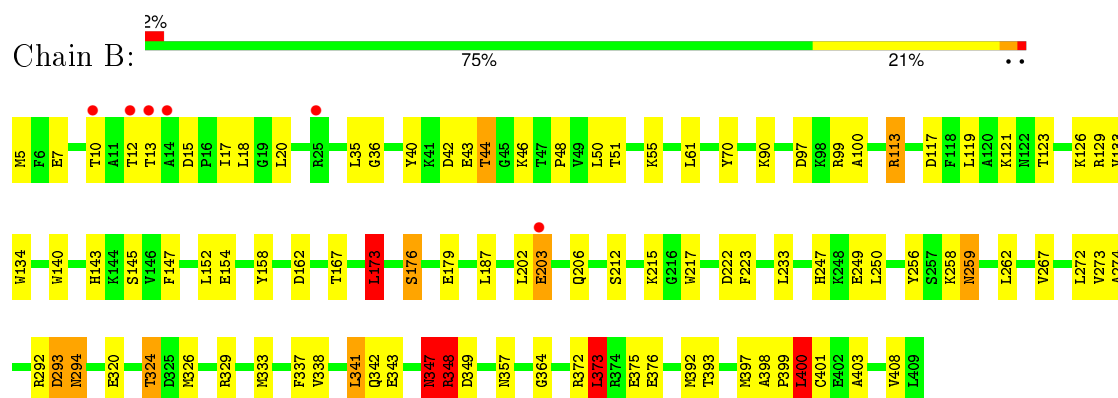
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ($\text{RSRZ} > 2$). 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: Aspartate aminotransferase



• Molecule 1: Aspartate aminotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	151.38 Å 151.38 Å 79.72 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.31 29.45 – 2.31	Depositor EDS
% Data completeness (in resolution range)	96.6 (30.00-2.31) 96.6 (29.45-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	11.74 (at 2.31 Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, R_{free}	0.185 , 0.232 0.185 , 0.229	Depositor DCC
R_{free} test set	2247 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.6	EDS
Estimated twinning fraction	0.023 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 44478 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6329	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: HCl, LLP

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	0.64	0/3120	0.81	4/4225 (0.1%)
1	B	0.73	0/3120	0.90	11/4225 (0.3%)
All	All	0.69	0/6240	0.86	15/8450 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	400	LEU	CA-CB-CG	8.03	133.78	115.30
1	B	97	ASP	CB-CG-OD2	6.87	124.48	118.30
1	B	293	ASP	CB-CG-OD2	6.51	124.16	118.30
1	B	222	ASP	CB-CG-OD2	6.30	123.97	118.30
1	B	173	LEU	CA-CB-CG	6.21	129.59	115.30
1	B	113	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	250	LEU	CA-CB-CG	5.75	128.52	115.30
1	B	15	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	313	ASP	CB-CG-OD2	5.51	123.26	118.30
1	B	341	LEU	CA-CB-CG	5.48	127.91	115.30
1	B	400	LEU	CB-CG-CD2	5.38	120.15	111.00
1	B	349	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	349	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	162	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	373	LEU	CA-CB-CG	5.15	127.14	115.30

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	3085	0	3019	39	0
1	B	3085	0	3019	83	0
2	A	11	0	9	0	0
2	B	11	0	9	0	0
3	A	60	0	0	4	0
3	B	77	0	0	4	0
All	All	6329	0	6056	116	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 9.

All (116) 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:333:MET:HE2	1:B:393:THR:CA	1.88	1.03
1:B:347:ASN:N	1:B:347:ASN:HD22	1.61	0.96
1:B:333:MET:HE2	1:B:393:THR:HA	1.48	0.94
1:B:397:MET:HE2	1:B:401:CYS:SG	2.15	0.87
1:A:336:LEU:O	1:A:340:THR:HG22	1.75	0.85
1:A:331:GLN:HG2	3:A:452:HOH:O	1.79	0.83
1:A:350:PHE:HB3	1:A:353:ILE:HD12	1.64	0.80
1:B:347:ASN:HD21	1:B:348:ARG:NH1	1.82	0.76
1:B:397:MET:CE	1:B:400:LEU:HD22	2.16	0.76
1:B:43:GLU:HG2	3:B:411:HOH:O	1.86	0.74
1:A:113:ARG:HD3	1:B:293:ASP:O	1.87	0.73
1:B:333:MET:HE2	1:B:393:THR:N	2.04	0.73
1:B:333:MET:CE	1:B:393:THR:CA	2.67	0.73
1:B:43:GLU:CG	3:B:411:HOH:O	2.37	0.72
1:B:397:MET:HE1	1:B:400:LEU:CD2	2.19	0.72
1:B:347:ASN:HD21	1:B:348:ARG:HH11	1.38	0.72
1:A:336:LEU:O	1:A:340:THR:CG2	2.36	0.72
1:B:162:ASP:HB3	1:B:167:THR:HG22	1.71	0.72
1:A:99:ARG:HD3	1:A:275:ALA:O	1.90	0.71
1:B:397:MET:CE	1:B:400:LEU:CD2	2.69	0.71
1:B:397:MET:HE1	1:B:400:LEU:HD21	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:ASN:N	1:B:347:ASN:ND2	2.33	0.68
1:A:211:LEU:HD13	1:A:217:TRP:CH2	2.28	0.68
1:B:348:ARG:HH11	1:B:348:ARG:HG3	1.58	0.68
1:A:294:ASN:HD21	1:B:294:ASN:HD21	1.42	0.68
1:A:99:ARG:HD2	1:A:274:ALA:O	1.97	0.64
1:B:40:TYR:CD2	1:B:326:MET:HE2	2.32	0.64
1:B:212:SER:OG	1:B:247:HIS:HE1	1.80	0.64
1:B:129:ARG:NH2	1:B:154:GLU:OE2	2.28	0.64
1:B:333:MET:HE2	1:B:392:MET:C	2.20	0.63
1:B:347:ASN:ND2	1:B:348:ARG:HH11	1.97	0.63
1:B:347:ASN:H	1:B:347:ASN:HD22	1.45	0.62
1:A:43:GLU:CD	1:A:43:GLU:H	2.02	0.62
1:B:42:ASP:OD1	1:B:44:THR:CG2	2.49	0.61
1:B:333:MET:CE	1:B:393:THR:N	2.64	0.60
1:B:397:MET:HA	1:B:400:LEU:HD13	1.84	0.59
1:A:237:ALA:O	1:A:241:ARG:HG3	2.02	0.59
1:B:48:PRO:HD2	3:B:434:HOH:O	2.04	0.57
1:B:333:MET:CE	1:B:392:MET:C	2.72	0.57
1:B:333:MET:HE1	1:B:393:THR:C	2.25	0.57
1:B:397:MET:CE	1:B:401:CYS:SG	2.90	0.56
1:A:256:TYR:HA	1:A:259:ASN:HD21	1.69	0.56
1:B:333:MET:CE	1:B:393:THR:C	2.75	0.55
1:B:212:SER:OG	1:B:247:HIS:CE1	2.59	0.55
1:B:397:MET:HE3	1:B:400:LEU:HD22	1.88	0.55
1:B:347:ASN:ND2	1:B:348:ARG:NH1	2.52	0.54
1:B:392:MET:HG2	1:B:400:LEU:HD11	1.89	0.54
1:B:176:SER:O	1:B:179:GLU:HG3	2.07	0.53
1:B:43:GLU:HG3	1:B:329:ARG:HD2	1.91	0.53
1:B:348:ARG:CG	1:B:348:ARG:HH11	2.19	0.53
1:B:42:ASP:OD1	1:B:44:THR:HG22	2.09	0.53
1:B:42:ASP:OD1	1:B:44:THR:HG23	2.08	0.53
1:A:142:ASN:ND2	1:B:292:ARG:HE	2.06	0.53
1:B:51:THR:O	1:B:55:LYS:HG3	2.09	0.52
1:A:331:GLN:CG	3:A:452:HOH:O	2.50	0.52
1:A:15:ASP:HB3	1:A:18:LEU:HB2	1.92	0.51
1:B:5:MET:N	1:B:7:GLU:OE1	2.43	0.51
1:B:99:ARG:HG2	1:B:274:ALA:O	2.11	0.51
1:B:347:ASN:CG	1:B:348:ARG:H	2.14	0.51
1:B:397:MET:HE3	1:B:397:MET:HA	1.92	0.50
1:B:113:ARG:HD2	1:B:117:ASP:OD2	2.10	0.50
1:B:250:LEU:HD12	1:B:273:VAL:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:ILE:O	1:B:20:LEU:HB2	2.10	0.50
1:A:189:HIS:HD2	3:A:416:HOH:O	1.95	0.50
1:B:337:PHE:HD1	1:B:397:MET:HE2	1.77	0.49
1:A:42:ASP:HB2	1:A:43:GLU:OE1	2.11	0.49
1:B:347:ASN:H	1:B:347:ASN:ND2	2.04	0.48
1:B:158:TYR:CD1	1:B:173:LEU:HD13	2.48	0.48
1:A:211:LEU:CD1	1:A:217:TRP:CH2	2.95	0.48
1:A:344:LYS:HE3	1:A:402:GLU:HG3	1.95	0.47
1:A:398:ALA:N	1:A:399:PRO:HD2	2.30	0.47
1:B:113:ARG:NH2	3:B:444:HOH:O	2.48	0.46
1:B:143:HIS:O	1:B:147:PHE:CD2	2.67	0.46
1:A:388:ASN:HD21	1:A:390:ALA:HB3	1.80	0.46
1:A:5:MET:N	1:B:249:GLU:OE1	2.48	0.46
1:A:309:ILE:O	1:A:316:ARG:HB3	2.16	0.46
1:B:40:TYR:CD2	1:B:326:MET:CE	2.99	0.46
1:B:40:TYR:CE2	1:B:326:MET:HG2	2.51	0.45
1:A:162:ASP:HB2	1:A:169:ASP:HB2	1.98	0.45
1:B:372:ARG:HG2	1:B:408:VAL:HG12	1.98	0.45
1:B:256:TYR:HA	1:B:259:ASN:HD21	1.82	0.45
1:A:113:ARG:HD2	1:A:113:ARG:HA	1.71	0.44
1:B:140:TRP:CD2	1:B:258:LLP:H2'3	2.51	0.44
1:B:215:LYS:HD2	1:B:217:TRP:CZ2	2.53	0.44
1:A:5:MET:SD	1:B:123:THR:HB	2.57	0.44
1:A:264:ASN:HD22	1:A:264:ASN:C	2.19	0.44
1:B:250:LEU:CD1	1:B:273:VAL:HG13	2.49	0.43
1:A:50:LEU:HD13	1:A:261:ALA:HB3	2.00	0.43
1:B:134:TRP:CH2	1:B:179:GLU:HB2	2.54	0.43
1:B:46:LYS:O	1:B:48:PRO:HD3	2.19	0.43
1:B:203:GLU:HG2	1:B:203:GLU:H	1.61	0.42
1:A:206:GLN:O	1:A:210:GLN:HG3	2.19	0.42
1:B:320:GLU:O	1:B:324:THR:HG23	2.20	0.42
1:B:100:ALA:HA	1:B:272:LEU:O	2.20	0.42
1:B:333:MET:HE2	1:B:392:MET:O	2.20	0.42
1:B:373:LEU:HD12	1:B:403:ALA:HB1	2.01	0.42
1:A:256:TYR:HA	1:A:259:ASN:ND2	2.34	0.42
1:A:189:HIS:HE1	3:A:437:HOH:O	2.03	0.42
1:A:5:MET:O	1:A:5:MET:HG3	2.19	0.42
1:B:187:LEU:C	1:B:187:LEU:HD23	2.41	0.42
1:B:35:LEU:HD11	1:B:400:LEU:HG	2.01	0.42
1:A:250:LEU:HB3	1:A:273:VAL:HB	2.02	0.42
1:A:160:TYR:O	1:A:168:LEU:HD23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:ALA:N	1:B:399:PRO:HD2	2.35	0.41
1:B:20:LEU:HD23	1:B:36:GLY:HA3	2.02	0.41
1:B:117:ASP:HB3	1:B:121:LYS:HE3	2.03	0.41
1:A:344:LYS:HB3	1:A:405:VAL:HG21	2.03	0.41
1:B:348:ARG:CG	1:B:348:ARG:NH1	2.81	0.41
1:B:202:LEU:O	1:B:206:GLN:HG3	2.21	0.40
1:B:7:GLU:CD	1:B:7:GLU:H	2.24	0.40
1:A:196:THR:O	1:A:356:GLN:HG2	2.22	0.40
1:A:212:SER:HB3	1:A:217:TRP:HE3	1.85	0.40
1:B:372:ARG:HD2	1:B:376:GLU:OE1	2.22	0.40
1:B:262:LEU:HD13	1:B:267:VAL:HG21	2.04	0.40
1:A:263:TYR:HB3	1:B:70:TYR:CZ	2.57	0.40
1:A:265:GLU:HA	1:A:265:GLU:OE1	2.21	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	393/396 (99%)	378 (96%)	14 (4%)	1 (0%)	46	56
1	B	393/396 (99%)	377 (96%)	13 (3%)	3 (1%)	24	27
All	All	786/792 (99%)	755 (96%)	27 (3%)	4 (0%)	34	40

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	ALA
1	B	348	ARG
1	B	347	ASN
1	B	364	GLY

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	320/320 (100%)	289 (90%)	31 (10%)	10	11
1	B	320/320 (100%)	289 (90%)	31 (10%)	10	11
All	All	640/640 (100%)	578 (90%)	62 (10%)	10	11

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	THR
1	A	13	THR
1	A	18	LEU
1	A	25	ARG
1	A	50	LEU
1	A	61	LEU
1	A	81	ARG
1	A	87	LEU
1	A	90	LYS
1	A	119	LEU
1	A	129	ARG
1	A	167	THR
1	A	168	LEU
1	A	179	GLU
1	A	202	LEU
1	A	211	LEU
1	A	212	SER
1	A	218	LEU
1	A	223	PHE
1	A	240	LEU
1	A	248	LYS
1	A	259	ASN
1	A	264	ASN
1	A	272	LEU
1	A	278	GLU
1	A	296	SER
1	A	316	ARG

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Mol	Chain	Res	Type
1	A	338	VAL
1	A	340	THR
1	A	341	LEU
1	A	365	LEU
1	B	10	THR
1	B	12	THR
1	B	13	THR
1	B	18	LEU
1	B	44	THR
1	B	50	LEU
1	B	61	LEU
1	B	90	LYS
1	B	119	LEU
1	B	126	LYS
1	B	133	VAL
1	B	145	SER
1	B	152	LEU
1	B	173	LEU
1	B	176	SER
1	B	203	GLU
1	B	223	PHE
1	B	233	LEU
1	B	259	ASN
1	B	294	ASN
1	B	324	THR
1	B	338	VAL
1	B	341	LEU
1	B	342	GLN
1	B	343	GLU
1	B	347	ASN
1	B	348	ARG
1	B	357	ASN
1	B	373	LEU
1	B	375	GLU
1	B	400	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	142	ASN
1	A	189	HIS

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Mol	Chain	Res	Type
1	A	206	GLN
1	A	226	GLN
1	A	259	ASN
1	A	264	ASN
1	A	328	GLN
1	A	357	ASN
1	A	388	ASN
1	B	84	GLN
1	B	175	ASN
1	B	206	GLN
1	B	226	GLN
1	B	247	HIS
1	B	259	ASN
1	B	294	ASN
1	B	328	GLN
1	B	339	ASN
1	B	342	GLN
1	B	347	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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	$\# Z > 2$
1	LLP	A	258	1	23,24,25	1.75	4 (17%)	28,32,34	2.19	7 (25%)
1	LLP	B	258	1	23,24,25	1.61	4 (17%)	28,32,34	2.21	8 (28%)

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
1	LLP	A	258	1	-	0/15/17/19	0/1/1/1
1	LLP	B	258	1	-	0/15/17/19	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	258	LLP	O3-C3	-5.26	1.24	1.37
1	B	258	LLP	O3-C3	-4.79	1.25	1.37
1	B	258	LLP	P-OP3	-2.29	1.46	1.54
1	B	258	LLP	C4-C4'	2.25	1.50	1.46
1	A	258	LLP	C2-N1	2.64	1.39	1.34
1	A	258	LLP	CE-NZ	2.71	1.52	1.46
1	B	258	LLP	CE-NZ	2.77	1.52	1.46
1	A	258	LLP	C4-C4'	2.95	1.51	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	LLP	C5-C4-C4'	-4.22	115.45	121.52
1	B	258	LLP	CE-NZ-C4'	-3.72	108.23	118.97
1	A	258	LLP	CE-NZ-C4'	-2.78	110.95	118.97
1	B	258	LLP	C5-C6-N1	-2.74	119.11	123.86
1	A	258	LLP	C5-C4-C4'	-2.68	117.65	121.52
1	A	258	LLP	O-C-CA	-2.53	118.91	125.49
1	B	258	LLP	O-C-CA	-2.23	119.69	125.49
1	A	258	LLP	C5-C6-N1	-2.20	120.03	123.86
1	B	258	LLP	C4-C4'-NZ	-2.16	113.03	125.06
1	A	258	LLP	C4-C4'-NZ	-2.08	113.50	125.06
1	A	258	LLP	C3-C4-C4'	2.25	123.07	120.16
1	B	258	LLP	C3-C4-C5	2.25	119.79	118.11
1	B	258	LLP	C3-C4-C4'	3.56	124.77	120.16
1	B	258	LLP	OP4-C5'-C5	7.16	120.83	108.99
1	A	258	LLP	OP4-C5'-C5	9.09	124.01	108.99

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
1	B	258	LLP	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are 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	HCI	A	410	-	8,11,11	0.84	0	10,13,13	0.73	0
2	HCI	B	410	-	8,11,11	1.23	0	10,13,13	0.49	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	HCI	A	410	-	-	0/3/5/5	0/1/1/1
2	HCI	B	410	-	-	0/3/5/5	0/1/1/1

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	395/396 (99%)	-0.12	13 (3%) 50 59	18, 26, 38, 46	0
1	B	395/396 (99%)	-0.41	6 (1%) 76 82	15, 24, 41, 51	0
All	All	790/792 (99%)	-0.27	19 (2%) 62 71	15, 25, 39, 51	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	14	ALA	5.4
1	A	347	ASN	4.2
1	B	12	THR	3.2
1	A	252	VAL	3.0
1	A	270	CYS	3.0
1	A	251	ILE	2.9
1	A	111	ALA	2.8
1	B	10	THR	2.8
1	A	25	ARG	2.7
1	A	253	ALA	2.5
1	A	90	LYS	2.5
1	A	224	ALA	2.4
1	A	269	ALA	2.4
1	B	25	ARG	2.4
1	B	203	GLU	2.3
1	A	271	THR	2.2
1	A	220	LEU	2.2
1	B	13	THR	2.2
1	A	254	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
1	LLP	A	258	24/25	0.98	0.18	-	18,23,25,26	0
1	LLP	B	258	24/25	0.98	0.10	-	15,18,19,22	0

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
2	HCI	A	410	11/11	0.96	0.13	0.02	20,22,24,26	0
2	HCI	B	410	11/11	0.97	0.08	-0.91	14,18,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.