



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 29, 2024 – 04:14 PM JST

PDB ID : 5WT5
Title : L-homocysteine-bound NifS from *Helicobacter pylori*
Authors : Fujishiro, T.; Takahashi, Y.
Deposited on : 2016-12-09
Resolution : 1.90 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

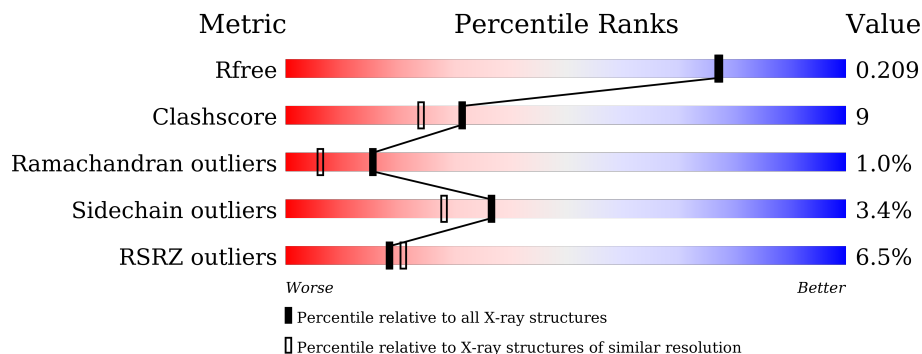
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	401	 5% 74% 16% • 9%
1	B	401	 6% 71% 17% • 9%
1	C	401	 6% 72% 16% • 9%
1	D	401	 6% 73% 16% • 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HCS	D	501	-	X	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12116 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 Cysteine desulfurase IscS.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	363	2826	1782	494	537	1	12	0	1	0
1	B	363	2822	1780	494	535	1	12	0	0	0
1	C	364	2829	1783	495	538	1	12	0	0	0
1	D	365	2834	1786	496	539	1	12	0	0	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	VAL	LEU	engineered mutation	UNP O25008
A	138	ARG	LYS	engineered mutation	UNP O25008
A	388	VAL	-	expression tag	UNP O25008
A	389	ASP	-	expression tag	UNP O25008
A	390	LEU	-	expression tag	UNP O25008
A	391	VAL	-	expression tag	UNP O25008
A	392	PRO	-	expression tag	UNP O25008
A	393	ARG	-	expression tag	UNP O25008
A	394	GLY	-	expression tag	UNP O25008
A	395	SER	-	expression tag	UNP O25008
A	396	HIS	-	expression tag	UNP O25008
A	397	HIS	-	expression tag	UNP O25008
A	398	HIS	-	expression tag	UNP O25008
A	399	HIS	-	expression tag	UNP O25008
A	400	HIS	-	expression tag	UNP O25008
A	401	HIS	-	expression tag	UNP O25008
B	2	VAL	LEU	engineered mutation	UNP O25008
B	138	ARG	LYS	engineered mutation	UNP O25008
B	388	VAL	-	expression tag	UNP O25008
B	389	ASP	-	expression tag	UNP O25008
B	390	LEU	-	expression tag	UNP O25008

Continued on next page...

Continued from previous page...

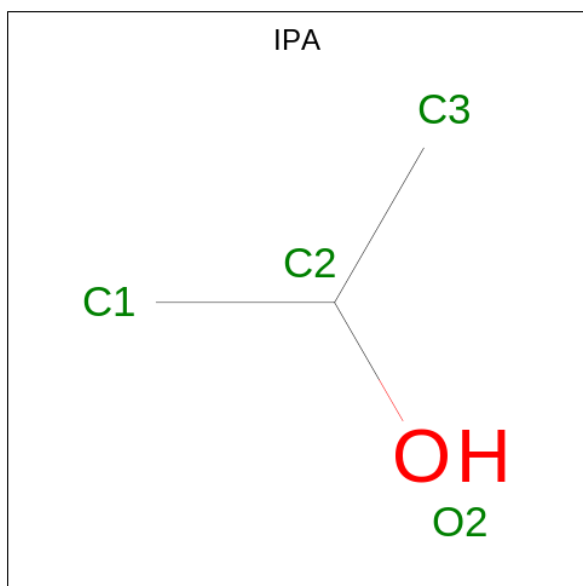
Chain	Residue	Modelled	Actual	Comment	Reference
B	391	VAL	-	expression tag	UNP O25008
B	392	PRO	-	expression tag	UNP O25008
B	393	ARG	-	expression tag	UNP O25008
B	394	GLY	-	expression tag	UNP O25008
B	395	SER	-	expression tag	UNP O25008
B	396	HIS	-	expression tag	UNP O25008
B	397	HIS	-	expression tag	UNP O25008
B	398	HIS	-	expression tag	UNP O25008
B	399	HIS	-	expression tag	UNP O25008
B	400	HIS	-	expression tag	UNP O25008
B	401	HIS	-	expression tag	UNP O25008
C	2	VAL	LEU	engineered mutation	UNP O25008
C	138	ARG	LYS	engineered mutation	UNP O25008
C	388	VAL	-	expression tag	UNP O25008
C	389	ASP	-	expression tag	UNP O25008
C	390	LEU	-	expression tag	UNP O25008
C	391	VAL	-	expression tag	UNP O25008
C	392	PRO	-	expression tag	UNP O25008
C	393	ARG	-	expression tag	UNP O25008
C	394	GLY	-	expression tag	UNP O25008
C	395	SER	-	expression tag	UNP O25008
C	396	HIS	-	expression tag	UNP O25008
C	397	HIS	-	expression tag	UNP O25008
C	398	HIS	-	expression tag	UNP O25008
C	399	HIS	-	expression tag	UNP O25008
C	400	HIS	-	expression tag	UNP O25008
C	401	HIS	-	expression tag	UNP O25008
D	2	VAL	LEU	engineered mutation	UNP O25008
D	138	ARG	LYS	engineered mutation	UNP O25008
D	388	VAL	-	expression tag	UNP O25008
D	389	ASP	-	expression tag	UNP O25008
D	390	LEU	-	expression tag	UNP O25008
D	391	VAL	-	expression tag	UNP O25008
D	392	PRO	-	expression tag	UNP O25008
D	393	ARG	-	expression tag	UNP O25008
D	394	GLY	-	expression tag	UNP O25008
D	395	SER	-	expression tag	UNP O25008
D	396	HIS	-	expression tag	UNP O25008
D	397	HIS	-	expression tag	UNP O25008
D	398	HIS	-	expression tag	UNP O25008
D	399	HIS	-	expression tag	UNP O25008
D	400	HIS	-	expression tag	UNP O25008

Continued on next page...

Continued from previous page...

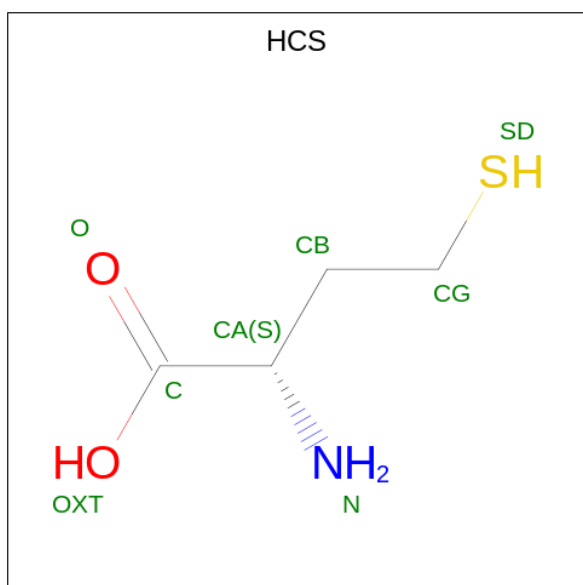
Chain	Residue	Modelled	Actual	Comment	Reference
D	401	HIS	-	expression tag	UNP O25008

- Molecule 2 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C₃H₈O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	3	1	0	0

- Molecule 3 is 2-AMINO-4-MERCAPTO-BUTYRIC ACID (three-letter code: HCS) (formula: C₄H₉NO₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			8	4	1	2	1		
3	B	1	Total	C	N	O	S	0	0
			8	4	1	2	1		
3	C	1	Total	C	N	O	S	0	0
			8	4	1	2	1		
3	D	1	Total	C	N	O	S	0	0
			8	4	1	2	1		

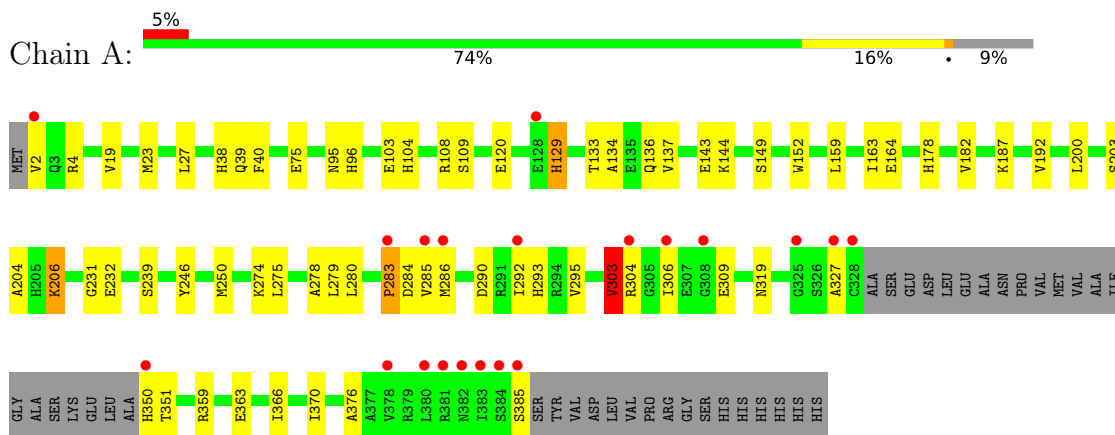
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	215	Total	O	0	0
			215	215		
4	B	175	Total	O	0	0
			175	175		
4	C	180	Total	O	0	0
			180	180		
4	D	199	Total	O	0	0
			199	199		

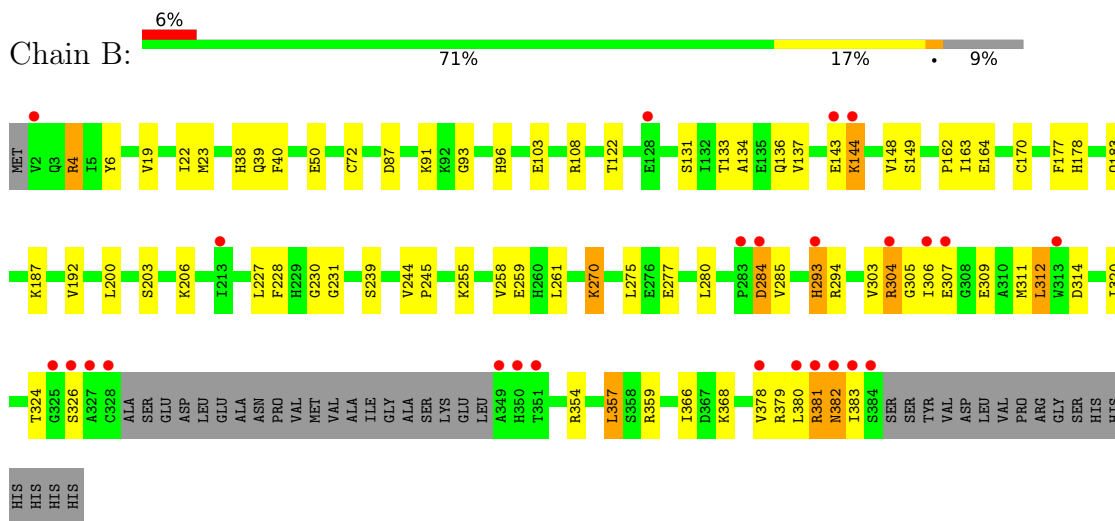
3 Residue-property plots [i](#)

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.

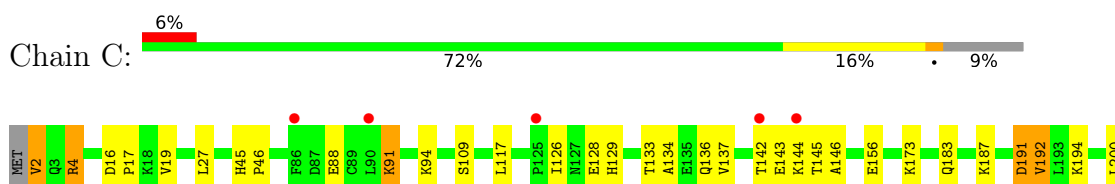
- Molecule 1: Cysteine desulfurase IscS

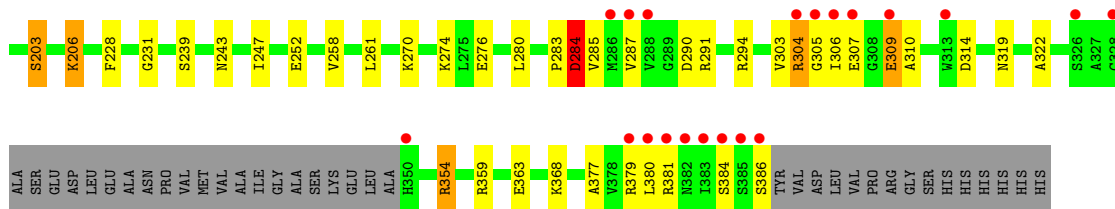


- Molecule 1: Cysteine desulfurase IscS

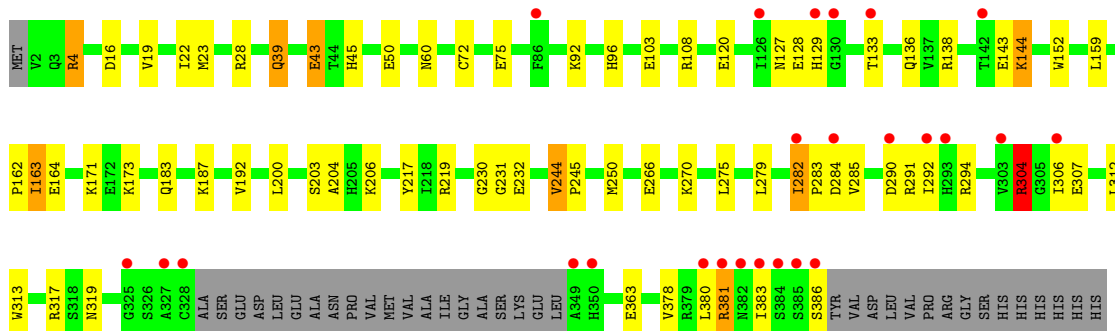
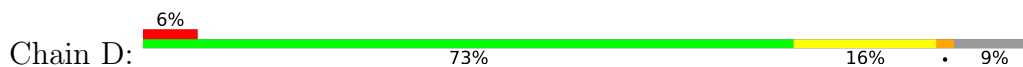


- Molecule 1: Cysteine desulfurase IscS





● Molecule 1: Cysteine desulfurase IscS



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.44Å 102.32Å 132.05Å 90.00° 90.10° 90.00°	Depositor
Resolution (Å)	47.78 – 1.90 47.78 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.78-1.90) 99.7 (47.78-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	23.88 (at 1.90Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.184 , 0.209 0.184 , 0.209	Depositor DCC
R_{free} test set	10809 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtrriage
Anisotropy	0.064	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.000 for k,h,-l 0.000 for -k,-h,-l 0.146 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12116	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HCS, LLP, IPA

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	0.93	2/2855 (0.1%)	0.97	7/3866 (0.2%)
1	B	0.92	4/2848 (0.1%)	0.97	7/3857 (0.2%)
1	C	0.94	4/2855 (0.1%)	0.98	9/3866 (0.2%)
1	D	0.86	3/2860 (0.1%)	0.92	7/3873 (0.2%)
All	All	0.91	13/11418 (0.1%)	0.96	30/15462 (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	C	0	1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	354	ARG	CZ-NH1	6.71	1.41	1.33
1	B	228	PHE	CD1-CE1	5.88	1.51	1.39
1	D	244	VAL	CB-CG2	5.50	1.64	1.52
1	A	75	GLU	CG-CD	5.46	1.60	1.51
1	B	228	PHE	CD2-CE2	5.46	1.50	1.39
1	D	217	TYR	CD1-CE1	-5.41	1.31	1.39
1	D	363	GLU	CG-CD	-5.34	1.44	1.51
1	C	192	VAL	CB-CG1	-5.25	1.41	1.52
1	B	244	VAL	CB-CG2	5.17	1.63	1.52
1	B	6	TYR	CD1-CE1	5.15	1.47	1.39
1	A	2	VAL	CB-CG1	5.13	1.63	1.52
1	C	88	GLU	CG-CD	5.12	1.59	1.51
1	C	252	GLU	CD-OE1	-5.02	1.20	1.25

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	359	ARG	NE-CZ-NH2	-9.10	115.75	120.30
1	B	359	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	B	354	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	C	359	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	B	312	LEU	CB-CG-CD1	-7.58	98.12	111.00
1	A	359	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	B	357	LEU	CB-CG-CD2	-7.07	98.98	111.00
1	C	4	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	B	359	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	D	4	ARG	NE-CZ-NH1	-6.24	117.18	120.30
1	C	4	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	D	144	LYS	N-CA-C	-6.18	94.30	111.00
1	A	182	VAL	CG1-CB-CG2	6.04	120.56	110.90
1	C	284	ASP	CB-CG-OD1	6.01	123.70	118.30
1	B	227	LEU	CB-CG-CD2	-5.91	100.96	111.00
1	A	359	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	D	363	GLU	CA-CB-CG	-5.74	100.78	113.40
1	C	354	ARG	CG-CD-NE	-5.68	99.88	111.80
1	B	294	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	D	291	ARG	NE-CZ-NH1	-5.59	117.51	120.30
1	A	303	VAL	CG1-CB-CG2	5.53	119.75	110.90
1	A	303	VAL	CA-CB-CG1	5.50	119.15	110.90
1	D	312	LEU	CA-CB-CG	5.50	127.94	115.30
1	C	27	LEU	CB-CG-CD1	-5.46	101.72	111.00
1	A	27	LEU	CB-CG-CD1	-5.44	101.75	111.00
1	D	291	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	A	246	TYR	CB-CG-CD1	5.32	124.19	121.00
1	D	28	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	C	191	ASP	CB-CG-OD2	5.04	122.83	118.30
1	C	117	LEU	CB-CG-CD2	-5.01	102.48	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	143	GLU	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	2826	0	2830	62	0
1	B	2822	0	2825	55	0
1	C	2829	0	2830	57	0
1	D	2834	0	2835	39	0
2	A	4	0	8	0	0
3	A	8	0	8	2	0
3	B	8	0	8	0	0
3	C	8	0	9	3	0
3	D	8	0	8	0	0
4	A	215	0	0	7	0
4	B	175	0	0	6	0
4	C	180	0	0	11	0
4	D	199	0	0	8	0
All	All	12116	0	11361	205	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 (205) 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:4:ARG:HH11	1:B:39:GLN:HE22	0.96	0.92
1:B:148:VAL:HG11	1:B:170:CYS:SG	2.16	0.86
1:C:307:GLU:HG2	1:C:310:ALA:H	1.41	0.86
1:C:306:ILE:HD11	1:C:381:ARG:HG2	1.58	0.85
1:A:4:ARG:HH11	1:B:39:GLN:NE2	1.74	0.85
1:A:129:HIS:HD2	1:A:290:ASP:HB2	1.44	0.82
1:A:4:ARG:NH1	1:B:39:GLN:HE22	1.76	0.82
1:C:307:GLU:OE1	4:C:601:HOH:O	2.00	0.78
1:A:231:GLY:N	1:A:239:SER:OG	2.16	0.78
1:D:284:ASP:OD2	1:D:304:ARG:HB3	1.84	0.78
1:A:95:ASN:HB3	1:A:144:LYS:NZ	1.98	0.77
1:C:231:GLY:N	1:C:239:SER:OG	2.19	0.75
1:C:285:VAL:HG22	1:C:303:VAL:HG12	1.68	0.75
1:D:183:GLN:O	1:D:187:LYS:HD2	1.87	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:HIS:HE2	3:A:502:HCS:HG2	1.53	0.73
1:D:284:ASP:OD1	1:D:304:ARG:HD2	1.90	0.72
1:A:280:LEU:O	4:A:601:HOH:O	2.08	0.71
1:A:303:VAL:CG1	1:A:306:ILE:HB	2.20	0.70
1:A:133:THR:HG22	1:A:136:GLN:HG3	1.74	0.70
1:B:381:ARG:HH21	1:B:381:ARG:HG2	1.57	0.70
1:A:164:GLU:HG2	4:A:782:HOH:O	1.91	0.69
1:A:284:ASP:HB2	1:A:304:ARG:CB	2.22	0.69
1:C:287:VAL:HG21	1:C:291:ARG:HD2	1.74	0.68
1:B:284:ASP:HB2	1:B:304:ARG:HB2	1.75	0.68
1:A:95:ASN:HB3	1:A:144:LYS:HZ1	1.58	0.68
1:A:284:ASP:HB2	1:A:304:ARG:HB2	1.76	0.68
1:C:307:GLU:OE2	1:C:310:ALA:HB2	1.95	0.66
1:B:258:VAL:HG21	4:B:745:HOH:O	1.95	0.66
1:D:304:ARG:HG3	1:D:306:ILE:HD12	1.78	0.66
1:D:378:VAL:O	1:D:381:ARG:HG3	1.96	0.65
1:B:285:VAL:HG22	1:B:303:VAL:HG12	1.79	0.65
1:A:275:LEU:HA	1:A:370:ILE:HD11	1.79	0.64
1:C:109:SER:HB3	1:D:230:GLY:HA2	1.80	0.63
1:A:385:SER:OG	4:A:602:HOH:O	2.16	0.63
1:A:129:HIS:HD2	1:A:290:ASP:CB	2.10	0.63
1:A:134:ALA:O	1:A:137:VAL:HG22	1.99	0.62
1:C:4:ARG:HB3	1:C:319:ASN:HB3	1.82	0.62
1:D:16:ASP:HB3	1:D:19:VAL:HG23	1.83	0.61
1:D:103:GLU:HB2	1:D:108:ARG:HG3	1.81	0.61
1:B:231:GLY:N	1:B:239:SER:OG	2.34	0.61
1:C:307:GLU:CD	1:C:310:ALA:HB2	2.20	0.61
1:A:192:VAL:HG12	1:A:200:LEU:HD13	1.83	0.60
1:B:93:GLY:O	1:B:144:LYS:HE3	2.01	0.60
1:C:134:ALA:O	1:C:137:VAL:HG22	2.00	0.60
1:B:134:ALA:O	1:B:137:VAL:HG22	2.02	0.60
1:C:270:LYS:NZ	4:C:606:HOH:O	2.29	0.59
1:B:162:PRO:O	1:B:164:GLU:N	2.35	0.59
1:B:284:ASP:CB	1:B:304:ARG:HB2	2.33	0.59
1:A:159:LEU:HD21	1:A:290:ASP:HB3	1.85	0.59
1:A:275:LEU:HD12	1:A:370:ILE:HD13	1.85	0.59
1:A:274:LYS:HE3	1:A:363:GLU:OE1	2.04	0.58
1:B:277:GLU:HG2	4:B:755:HOH:O	2.02	0.58
1:B:381:ARG:HG3	1:B:382:ASN:N	2.19	0.58
1:C:287:VAL:HG22	4:C:638:HOH:O	2.04	0.58
1:C:314:ASP:CG	1:C:379:ARG:HH21	2.07	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:LYS:HE3	1:C:363:GLU:OE1	2.04	0.57
1:B:148:VAL:CG1	1:B:170:CYS:SG	2.92	0.57
1:B:183:GLN:O	1:B:187:LYS:HD2	2.05	0.57
1:B:378:VAL:HA	1:B:381:ARG:HG2	1.86	0.57
1:D:127:ASN:OD1	1:D:129:HIS:HB2	2.05	0.57
1:C:307:GLU:HG3	1:C:309:GLU:OE2	2.05	0.56
1:D:39:GLN:O	1:D:43:GLU:HB2	2.05	0.56
1:D:317:ARG:NH1	4:D:606:HOH:O	2.32	0.56
1:A:284:ASP:HB2	1:A:304:ARG:HB3	1.89	0.55
1:C:284:ASP:OD2	1:C:284:ASP:N	2.40	0.55
1:B:314:ASP:OD2	1:B:379:ARG:NH2	2.38	0.55
1:B:19:VAL:O	1:B:22:ILE:HG22	2.07	0.55
1:A:4:ARG:HB3	1:A:319:ASN:HB3	1.88	0.54
1:A:129:HIS:CD2	1:A:290:ASP:HB2	2.34	0.54
1:C:284:ASP:HB2	1:C:304:ARG:HB2	1.90	0.54
1:B:275:LEU:HD12	1:B:366:ILE:HD12	1.88	0.54
1:C:307:GLU:CG	1:C:310:ALA:H	2.17	0.54
1:D:313:TRP:CH2	1:D:317:ARG:HD2	2.43	0.53
1:A:96:HIS:HD2	1:A:120:GLU:HG2	1.74	0.53
1:B:96:HIS:NE2	1:B:122:THR:HG23	2.24	0.53
1:C:354:ARG:NH1	3:C:501:HCS:O	2.36	0.53
1:B:293:HIS:N	4:B:601:HOH:O	2.17	0.53
1:A:275:LEU:O	1:A:279:LEU:HG	2.09	0.52
1:B:307:GLU:HG3	1:B:309:GLU:OE1	2.09	0.52
1:C:17:PRO:HD2	4:C:608:HOH:O	2.09	0.52
1:A:103:GLU:HB2	1:A:108:ARG:HG3	1.90	0.52
1:B:87:ASP:HA	1:B:91:LYS:HD3	1.92	0.52
1:A:275:LEU:HD12	1:A:370:ILE:CD1	2.40	0.52
1:D:4:ARG:HB3	1:D:319:ASN:HB3	1.92	0.51
1:A:284:ASP:N	1:A:284:ASP:OD1	2.44	0.51
1:B:378:VAL:O	1:B:381:ARG:HG3	2.10	0.51
1:C:91:LYS:NZ	4:C:611:HOH:O	2.43	0.51
1:C:183:GLN:O	1:C:187:LYS:HD2	2.10	0.51
1:D:19:VAL:O	1:D:22:ILE:HG22	2.12	0.50
1:D:304:ARG:HG3	1:D:306:ILE:CD1	2.40	0.50
1:A:204:ALA:HB2	1:A:250:MET:SD	2.52	0.50
1:D:50:GLU:HG3	4:D:720:HOH:O	2.12	0.50
1:D:60:ASN:HB2	4:D:629:HOH:O	2.11	0.50
1:D:162:PRO:O	1:D:164:GLU:N	2.45	0.50
1:C:192:VAL:HG12	1:C:200:LEU:HD13	1.94	0.49
1:D:23:MET:HG2	1:D:245:PRO:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:ASP:OD1	1:D:292:ILE:N	2.34	0.49
1:B:23:MET:HG2	1:B:245:PRO:O	2.11	0.49
1:D:380:LEU:HA	1:D:383:ILE:HG22	1.93	0.49
1:B:50:GLU:HG3	4:B:740:HOH:O	2.12	0.49
1:B:312:LEU:HD11	1:B:324:THR:HG23	1.94	0.49
1:B:103:GLU:HB2	1:B:108:ARG:HG3	1.95	0.48
1:A:285:VAL:HG22	1:A:303:VAL:HG22	1.94	0.48
1:A:133:THR:HG23	1:A:136:GLN:H	1.78	0.48
1:A:4:ARG:NH1	1:B:39:GLN:NE2	2.47	0.48
1:A:39:GLN:OE1	1:B:4:ARG:NH1	2.47	0.48
1:C:203:SER:OG	1:C:206:LLP:OP3	2.27	0.48
1:B:258:VAL:HA	1:B:261:LEU:HG	1.96	0.48
1:C:133:THR:HG21	4:C:718:HOH:O	2.13	0.48
1:B:133:THR:HG22	1:B:136:GLN:HG3	1.96	0.48
1:A:159:LEU:CD2	1:A:290:ASP:HB3	2.43	0.47
1:B:381:ARG:HG3	1:B:382:ASN:H	1.78	0.47
1:C:142:THR:C	1:C:144:LYS:H	2.16	0.47
1:C:243:ASN:O	1:C:247:ILE:HG13	2.14	0.47
1:A:303:VAL:HG11	1:A:306:ILE:HB	1.95	0.47
1:C:287:VAL:HG21	1:C:291:ARG:CD	2.44	0.47
1:D:159:LEU:HD23	1:D:294:ARG:HB3	1.95	0.47
1:B:307:GLU:H	1:B:307:GLU:CD	2.19	0.46
1:A:366:ILE:O	1:A:370:ILE:HG12	2.16	0.46
1:C:287:VAL:HG21	1:C:291:ARG:CG	2.46	0.46
1:A:38:HIS:CE1	1:A:40:PHE:HB2	2.51	0.46
1:B:133:THR:HG23	1:B:136:GLN:H	1.80	0.46
1:B:255:LYS:HE2	1:B:259:GLU:OE2	2.15	0.46
1:C:377:ALA:O	1:C:381:ARG:HG3	2.16	0.46
1:C:91:LYS:HA	1:C:91:LYS:HD3	1.55	0.46
3:C:501:HCS:OXT	3:C:501:HCS:HG2	2.14	0.45
1:B:280:LEU:HD23	1:B:280:LEU:HA	1.85	0.45
1:C:191:ASP:OD1	1:C:194:LYS:HG3	2.16	0.45
1:C:290:ASP:OD1	1:C:291:ARG:N	2.50	0.45
1:A:303:VAL:HG12	1:A:306:ILE:O	2.17	0.45
1:B:314:ASP:CG	1:B:379:ARG:HH22	2.19	0.45
1:C:354:ARG:HH22	3:C:501:HCS:C	2.30	0.45
1:C:126:ILE:HG22	4:C:647:HOH:O	2.16	0.45
1:C:380:LEU:O	1:C:384:SER:HB2	2.17	0.45
1:A:285:VAL:HG22	1:A:303:VAL:CG2	2.46	0.44
1:C:94:LYS:O	1:C:146:ALA:HB2	2.17	0.44
1:A:327:ALA:HB3	1:A:350:HIS:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:ASP:CG	1:B:304:ARG:HB2	2.38	0.44
1:D:266:GLU:O	1:D:270:LYS:HG2	2.17	0.44
1:A:19:VAL:O	1:A:23:MET:HG3	2.18	0.44
1:B:164:GLU:HB2	4:B:602:HOH:O	2.17	0.44
1:C:142:THR:O	1:C:144:LYS:N	2.51	0.44
1:C:276:GLU:OE1	1:C:294:ARG:NH1	2.35	0.44
1:A:149:SER:HA	1:A:178:HIS:O	2.17	0.44
1:D:45:HIS:ND1	4:D:609:HOH:O	2.37	0.44
1:D:378:VAL:HA	1:D:381:ARG:HG2	1.98	0.44
1:D:92:LYS:HD3	4:D:734:HOH:O	2.17	0.43
1:D:282:ILE:HG13	1:D:285:VAL:HG21	2.00	0.43
1:A:95:ASN:HB3	1:A:144:LYS:HZ3	1.79	0.43
1:A:280:LEU:HD23	1:A:280:LEU:HA	1.82	0.43
1:A:376:ALA:HB2	4:A:700:HOH:O	2.18	0.43
1:C:2:VAL:N	4:C:627:HOH:O	2.51	0.43
1:A:133:THR:HG22	1:A:136:GLN:CG	2.45	0.43
1:B:380:LEU:HA	1:B:383:ILE:HG22	2.01	0.43
1:D:304:ARG:CG	1:D:306:ILE:HD12	2.47	0.43
1:A:133:THR:HG21	4:A:800:HOH:O	2.18	0.42
1:C:307:GLU:HG3	1:C:309:GLU:CG	2.49	0.42
1:A:303:VAL:HG13	1:A:306:ILE:HB	2.00	0.42
1:A:293:HIS:CE1	4:A:744:HOH:O	2.72	0.42
1:B:192:VAL:HG12	1:B:200:LEU:HD13	2.01	0.42
1:B:320:ILE:HD13	1:B:320:ILE:HG21	1.87	0.42
1:C:276:GLU:CD	1:C:294:ARG:HH12	2.18	0.42
1:D:152:TRP:HA	1:D:163:ILE:HD11	2.02	0.42
1:D:187:LYS:NZ	4:D:623:HOH:O	2.52	0.42
1:A:295:VAL:HG21	4:A:715:HOH:O	2.19	0.42
1:B:270:LYS:HG2	4:B:605:HOH:O	2.19	0.42
1:C:16:ASP:HB3	1:C:19:VAL:HG23	2.00	0.42
1:A:206:LLP:H4'1	3:A:502:HCS:HG3	2.02	0.42
1:A:280:LEU:HD21	1:A:286:MET:HA	2.01	0.42
1:C:142:THR:N	1:C:145:THR:OG1	2.45	0.42
1:D:231:GLY:N	4:D:624:HOH:O	2.53	0.42
1:A:309:GLU:OE2	1:A:351:THR:OG1	2.27	0.42
1:A:109[B]:SER:HB3	1:B:230:GLY:HA2	2.00	0.42
1:B:38:HIS:CE1	1:B:40:PHE:HB2	2.55	0.42
1:C:284:ASP:CB	1:C:304:ARG:HB2	2.50	0.42
1:D:244:VAL:HB	1:D:245:PRO:HD3	2.00	0.42
1:C:314:ASP:O	4:C:602:HOH:O	2.22	0.41
1:C:45:HIS:HB2	1:C:46:PRO:HD3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:LEU:HD23	1:C:280:LEU:HA	1.89	0.41
1:C:304:ARG:HG3	1:C:305:GLY:N	2.35	0.41
1:A:96:HIS:CD2	1:A:120:GLU:HG2	2.53	0.41
1:A:278:ALA:HB3	1:A:370:ILE:HD12	2.01	0.41
1:B:381:ARG:HG2	1:B:381:ARG:NH2	2.30	0.41
1:C:258:VAL:HA	1:C:261:LEU:HG	2.03	0.41
1:D:192:VAL:HG12	1:D:200:LEU:HD13	2.03	0.41
1:D:219:ARG:NH1	4:D:622:HOH:O	2.51	0.41
1:B:368:LYS:HD3	1:B:368:LYS:HA	1.76	0.41
1:D:204:ALA:HB2	1:D:250:MET:SD	2.61	0.41
1:A:292:ILE:HG22	1:A:293:HIS:N	2.36	0.41
1:C:156:GLU:HG2	4:C:696:HOH:O	2.21	0.41
1:A:109[A]:SER:HB2	1:B:230:GLY:HA2	2.02	0.41
1:C:294:ARG:HG2	4:C:605:HOH:O	2.20	0.41
1:D:96:HIS:HA	1:D:120:GLU:O	2.21	0.41
1:B:357:LEU:HD12	1:B:357:LEU:N	2.36	0.41
1:D:133:THR:OG1	1:D:136:GLN:HG3	2.21	0.41
1:C:133:THR:HG23	1:C:136:GLN:H	1.86	0.41
1:C:322:ALA:HB1	1:C:354:ARG:O	2.21	0.41
1:A:152:TRP:HA	1:A:163:ILE:HD11	2.03	0.40
1:B:149:SER:HA	1:B:178:HIS:O	2.21	0.40
1:B:148:VAL:HG13	1:B:177:PHE:HD1	1.86	0.40
1:C:228:PHE:CZ	1:D:75:GLU:HB2	2.56	0.40
1:B:381:ARG:NH2	1:B:381:ARG:CG	2.85	0.40
1:D:275:LEU:O	1:D:279:LEU:HG	2.20	0.40
1:C:133:THR:HG22	1:C:136:GLN:OE1	2.22	0.40
1:A:283:PRO:HB2	1:A:284:ASP:H	1.51	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	359/401 (90%)	347 (97%)	11 (3%)	1 (0%)	41	31
1	B	358/401 (89%)	346 (97%)	7 (2%)	5 (1%)	11	3
1	C	359/401 (90%)	346 (96%)	10 (3%)	3 (1%)	19	9
1	D	360/401 (90%)	347 (96%)	8 (2%)	5 (1%)	11	3
All	All	1436/1604 (90%)	1386 (96%)	36 (2%)	14 (1%)	15	6

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	283	PRO
1	B	304	ARG
1	C	304	ARG
1	D	163	ILE
1	D	304	ARG
1	B	163	ILE
1	C	283	PRO
1	D	283	PRO
1	B	284	ASP
1	C	284	ASP
1	B	72	CYS
1	D	72	CYS
1	D	232	GLU
1	B	305	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	306/336 (91%)	300 (98%)	6 (2%)	55	51
1	B	304/336 (90%)	292 (96%)	12 (4%)	32	23
1	C	306/336 (91%)	297 (97%)	9 (3%)	42	35
1	D	306/336 (91%)	292 (95%)	14 (5%)	27	17
All	All	1222/1344 (91%)	1181 (97%)	41 (3%)	37	28

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	HIS
1	A	143	GLU
1	A	187	LYS
1	A	203	SER
1	A	232	GLU
1	A	303	VAL
1	B	4	ARG
1	B	131	SER
1	B	143	GLU
1	B	144	LYS
1	B	203	SER
1	B	270	LYS
1	B	293	HIS
1	B	306	ILE
1	B	311	MET
1	B	326	SER
1	B	381	ARG
1	B	382	ASN
1	C	2	VAL
1	C	91	LYS
1	C	128	GLU
1	C	129	HIS
1	C	173	LYS
1	C	203	SER
1	C	309	GLU
1	C	368	LYS
1	C	386	SER
1	D	39	GLN
1	D	43	GLU
1	D	128	GLU
1	D	138	ARG
1	D	143	GLU
1	D	144	LYS
1	D	171	LYS
1	D	173	LYS
1	D	203	SER
1	D	282	ILE
1	D	304	ARG
1	D	307	GLU
1	D	381	ARG
1	D	386	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	HIS
1	B	39	GLN
1	B	95	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

4 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	B	206	1	23,24,25	2.58	6 (26%)	25,32,34	2.21	12 (48%)
1	LLP	A	206	1	23,24,25	2.62	7 (30%)	25,32,34	1.63	7 (28%)
1	LLP	C	206	1	23,24,25	2.80	6 (26%)	25,32,34	2.36	13 (52%)
1	LLP	D	206	1	23,24,25	3.01	9 (39%)	25,32,34	1.86	7 (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	B	206	1	-	2/16/17/19	0/1/1/1
1	LLP	A	206	1	-	3/16/17/19	0/1/1/1
1	LLP	C	206	1	-	3/16/17/19	0/1/1/1
1	LLP	D	206	1	-	4/16/17/19	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	206	LLP	C4'-NZ	8.77	1.56	1.27
1	C	206	LLP	C4-C4'	8.09	1.62	1.46
1	C	206	LLP	C4'-NZ	7.92	1.53	1.27
1	D	206	LLP	C4'-NZ	7.80	1.53	1.27
1	D	206	LLP	C4-C4'	7.66	1.61	1.46
1	A	206	LLP	C4-C4'	6.03	1.58	1.46
1	A	206	LLP	C4'-NZ	5.46	1.45	1.27
1	A	206	LLP	CB-CA	-5.37	1.46	1.53
1	D	206	LLP	C3-C2	4.94	1.45	1.40
1	B	206	LLP	C4-C4'	4.80	1.55	1.46
1	A	206	LLP	C3-C2	4.44	1.45	1.40
1	C	206	LLP	P-OP4	4.01	1.73	1.60
1	D	206	LLP	C2'-C2	3.82	1.56	1.50
1	D	206	LLP	CB-CA	-3.58	1.48	1.53
1	B	206	LLP	P-OP3	-3.56	1.41	1.54
1	B	206	LLP	P-OP1	2.82	1.59	1.50
1	A	206	LLP	C5'-C5	2.79	1.58	1.50
1	A	206	LLP	C2'-C2	2.65	1.54	1.50
1	D	206	LLP	P-OP2	-2.64	1.44	1.54
1	C	206	LLP	C4-C5	-2.63	1.38	1.42
1	B	206	LLP	C2'-C2	2.62	1.54	1.50
1	D	206	LLP	P-OP1	2.55	1.58	1.50
1	C	206	LLP	C4-C3	-2.52	1.37	1.40
1	B	206	LLP	CB-CA	-2.38	1.50	1.53
1	D	206	LLP	C5'-C5	2.34	1.57	1.50
1	C	206	LLP	P-OP2	-2.33	1.45	1.54
1	D	206	LLP	P-OP3	-2.22	1.46	1.54
1	A	206	LLP	C6-N1	2.01	1.38	1.34

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	206	LLP	OP3-P-OP4	-4.78	94.02	106.73
1	D	206	LLP	C3-C4-C5	-4.69	114.66	118.26
1	C	206	LLP	CD-CE-NZ	4.21	121.25	110.93
1	B	206	LLP	C5-C4-C4'	-3.96	115.05	121.56
1	B	206	LLP	C4-C3-C2	-3.93	117.75	120.19
1	C	206	LLP	C4-C4'-NZ	-3.85	106.64	124.31
1	B	206	LLP	OP4-C5'-C5	3.44	115.90	109.35
1	C	206	LLP	C5-C4-C4'	3.43	127.20	121.56
1	C	206	LLP	OP3-P-OP2	3.35	120.43	107.64
1	D	206	LLP	OP4-C5'-C5	3.33	115.70	109.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	206	LLP	OP4-P-OP1	-3.33	97.13	106.47
1	D	206	LLP	C5'-C5-C6	-3.28	113.98	119.37
1	A	206	LLP	C5'-C5-C6	-3.25	114.03	119.37
1	C	206	LLP	C2'-C2-C3	-3.06	117.11	120.89
1	B	206	LLP	CE-NZ-C4'	-3.02	109.62	118.90
1	B	206	LLP	C3-C4-C4'	2.94	125.90	120.41
1	B	206	LLP	OP3-P-OP4	2.85	114.31	106.73
1	D	206	LLP	C5-C4-C4'	2.84	126.22	121.56
1	A	206	LLP	C4-C4'-NZ	-2.79	111.48	124.31
1	A	206	LLP	C4-C3-C2	-2.72	118.50	120.19
1	C	206	LLP	C5'-C5-C6	-2.66	114.99	119.37
1	B	206	LLP	C5-C6-N1	-2.62	119.46	123.82
1	C	206	LLP	OP2-P-OP4	2.58	113.61	106.73
1	C	206	LLP	C6-C5-C4	2.55	122.84	118.15
1	D	206	LLP	C6-C5-C4	2.47	122.69	118.15
1	C	206	LLP	C3-C4-C4'	-2.43	115.88	120.41
1	B	206	LLP	C4-C4'-NZ	-2.43	113.17	124.31
1	A	206	LLP	OP3-P-OP2	2.36	116.65	107.64
1	D	206	LLP	OP3-P-OP4	-2.25	100.76	106.73
1	C	206	LLP	C5-C6-N1	-2.21	120.14	123.82
1	A	206	LLP	C5-C6-N1	-2.20	120.15	123.82
1	A	206	LLP	OP4-P-OP1	2.16	112.53	106.47
1	C	206	LLP	C3-C4-C5	-2.14	116.61	118.26
1	C	206	LLP	C3-C2-N1	2.12	123.50	120.77
1	B	206	LLP	CD-CG-CB	2.12	121.12	113.62
1	A	206	LLP	OP2-P-OP4	-2.10	101.14	106.73
1	B	206	LLP	CD-CE-NZ	2.05	115.96	110.93
1	D	206	LLP	OP3-P-OP2	2.03	115.41	107.64
1	B	206	LLP	O3-C3-C4	2.02	125.03	119.60

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	206	LLP	C-CA-CB-CG
1	D	206	LLP	C-CA-CB-CG
1	A	206	LLP	C4-C4'-NZ-CE
1	B	206	LLP	C4-C4'-NZ-CE
1	C	206	LLP	C4-C4'-NZ-CE
1	D	206	LLP	C4-C4'-NZ-CE
1	B	206	LLP	C5'-OP4-P-OP1
1	D	206	LLP	C5'-OP4-P-OP1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	C	206	LLP	C3-C4-C4'-NZ
1	C	206	LLP	C-CA-CB-CG
1	A	206	LLP	C3-C4-C4'-NZ
1	D	206	LLP	C3-C4-C4'-NZ

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	206	LLP	1	0
1	C	206	LLP	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	IPA	A	501	-	3,3,3	0.53	0	3,3,3	0.53	0
3	HCS	C	501	-	6,7,7	1.18	1 (16%)	7,8,8	3.74	4 (57%)
3	HCS	B	501	-	6,7,7	2.23	2 (33%)	7,8,8	2.64	3 (42%)
3	HCS	D	501	-	6,7,7	2.20	2 (33%)	7,8,8	2.59	4 (57%)
3	HCS	A	502	-	6,7,7	1.25	1 (16%)	7,8,8	4.23	4 (57%)

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
3	HCS	B	501	-	-	2/7/7/7	-
3	HCS	D	501	-	-	3/7/7/7	-
3	HCS	C	501	-	-	1/7/7/7	-
3	HCS	A	502	-	-	3/7/7/7	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	501	HCS	O-C	4.68	1.36	1.22
3	B	501	HCS	O-C	4.44	1.35	1.22
3	B	501	HCS	OXT-C	-2.61	1.22	1.30
3	C	501	HCS	OXT-C	2.29	1.38	1.30
3	D	501	HCS	OXT-C	-2.22	1.23	1.30
3	A	502	HCS	CB-CG	-2.08	1.50	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	HCS	CB-CG-SD	-10.16	103.16	113.74
3	C	501	HCS	CB-CG-SD	-7.75	105.67	113.74
3	C	501	HCS	OXT-C-O	-4.59	113.66	124.09
3	B	501	HCS	OXT-C-O	-4.21	114.52	124.09
3	D	501	HCS	OXT-C-CA	4.08	127.28	113.38
3	B	501	HCS	CB-CG-SD	-3.92	109.65	113.74
3	B	501	HCS	OXT-C-CA	3.48	125.22	113.38
3	D	501	HCS	O-C-CA	-3.03	111.44	122.14
3	D	501	HCS	CB-CA-N	3.02	118.08	110.17
3	C	501	HCS	OXT-C-CA	3.01	123.63	113.38
3	D	501	HCS	CB-CG-SD	-2.79	110.83	113.74
3	A	502	HCS	OXT-C-O	-2.56	118.27	124.09
3	A	502	HCS	CB-CA-N	2.30	116.21	110.17
3	C	501	HCS	CB-CA-N	2.16	115.82	110.17
3	A	502	HCS	CB-CA-C	-2.14	105.20	110.30

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	HCS	O-C-CA-N
3	D	501	HCS	O-C-CA-N
3	D	501	HCS	CA-CB-CG-SD

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	501	HCS	OXT-C-CA-N
3	A	502	HCS	OXT-C-CA-N
3	B	501	HCS	CA-CB-CG-SD
3	C	501	HCS	CA-CB-CG-SD
3	B	501	HCS	C-CA-CB-CG
3	A	502	HCS	CA-CB-CG-SD

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	501	HCS	3	0
3	A	502	HCS	2	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

6.1 Protein, DNA and RNA chains

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	362/401 (90%)	0.39	20 (5%) 25 28	19, 36, 66, 97	0
1	B	362/401 (90%)	0.43	25 (6%) 16 19	21, 35, 64, 79	0
1	C	363/401 (90%)	0.47	25 (6%) 16 19	19, 37, 64, 108	0
1	D	364/401 (90%)	0.53	25 (6%) 16 19	21, 39, 64, 81	0
All	All	1451/1604 (90%)	0.45	95 (6%) 18 21	19, 37, 65, 108	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	386	SER	8.8
1	D	384	SER	8.2
1	B	383	ILE	8.0
1	C	383	ILE	7.8
1	C	384	SER	7.4
1	C	328	CYS	7.4
1	C	304	ARG	6.9
1	C	386	SER	6.9
1	B	350	HIS	6.8
1	A	384	SER	6.7
1	A	383	ILE	6.6
1	B	304	ARG	6.6
1	B	349	ALA	6.6
1	D	328	CYS	6.3
1	C	385	SER	6.3
1	D	382	ASN	6.2
1	C	381	ARG	6.2
1	D	385	SER	6.1
1	D	383	ILE	6.1
1	A	328	CYS	5.8
1	D	126	ILE	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	384	SER	5.5
1	D	349	ALA	5.4
1	A	381	ARG	5.1
1	A	382	ASN	5.0
1	D	381	ARG	4.8
1	B	306	ILE	4.7
1	A	327	ALA	4.7
1	A	385	SER	4.6
1	A	378	VAL	4.5
1	C	307	GLU	4.5
1	A	350	HIS	4.5
1	A	306	ILE	4.2
1	B	381	ARG	4.1
1	B	328	CYS	4.0
1	C	382	ASN	4.0
1	B	382	ASN	4.0
1	B	327	ALA	4.0
1	B	378	VAL	3.9
1	C	142	THR	3.7
1	D	325	GLY	3.6
1	A	283	PRO	3.6
1	D	380	LEU	3.6
1	B	283	PRO	3.6
1	C	286	MET	3.6
1	D	327	ALA	3.6
1	C	313	TRP	3.5
1	D	133	THR	3.4
1	D	306	ILE	3.3
1	C	350	HIS	3.2
1	D	350	HIS	3.2
1	B	128	GLU	3.2
1	D	142	THR	3.1
1	C	326	SER	3.0
1	B	325	GLY	3.0
1	B	380	LEU	2.9
1	C	86	PHE	2.9
1	D	86	PHE	2.9
1	D	303	VAL	2.9
1	A	304	ARG	2.9
1	C	125	PRO	2.8
1	C	305	GLY	2.8
1	D	130	GLY	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	379	ARG	2.8
1	B	143	GLU	2.7
1	B	284	ASP	2.7
1	A	380	LEU	2.6
1	C	288	VAL	2.6
1	C	90	LEU	2.5
1	D	284	ASP	2.5
1	A	2	VAL	2.5
1	B	144	LYS	2.5
1	B	307	GLU	2.5
1	C	144	LYS	2.4
1	B	313	TRP	2.4
1	A	128	GLU	2.4
1	A	308	GLY	2.4
1	D	292	ILE	2.4
1	D	293	HIS	2.3
1	D	129	HIS	2.3
1	D	290	ASP	2.3
1	B	351	THR	2.3
1	C	287	VAL	2.3
1	C	309	GLU	2.2
1	A	292	ILE	2.2
1	B	293	HIS	2.1
1	C	380	LEU	2.1
1	B	213	ILE	2.1
1	A	285	VAL	2.1
1	D	282	ILE	2.1
1	B	2	VAL	2.1
1	A	325	GLY	2.1
1	A	286	MET	2.0
1	B	326	SER	2.0
1	C	306	ILE	2.0

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. 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
1	LLP	D	206	24/25	0.96	0.15	21,26,34,41	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	LLP	C	206	24/25	0.97	0.14	18,24,43,45	0
1	LLP	A	206	24/25	0.97	0.13	20,24,29,33	0
1	LLP	B	206	24/25	0.98	0.13	20,25,34,35	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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(\AA^2)	Q<0.9
3	HCS	C	501	8/8	0.81	0.14	44,46,51,54	0
2	IPA	A	501	4/4	0.82	0.23	60,64,65,67	0
3	HCS	A	502	8/8	0.83	0.13	44,48,50,55	0
3	HCS	D	501	8/8	0.88	0.11	49,53,56,59	0
3	HCS	B	501	8/8	0.93	0.15	37,43,48,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.