



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:54 AM UTC

PDB ID : 1GSS / pdb_00001gss
Title : THREE-DIMENSIONAL STRUCTURE OF CLASS PI GLUTATHIONE S-TRANSFERASE FROM HUMAN PLACENTA IN COMPLEX WITH S-HEXYLGLUTATHIONE AT 2.8 ANGSTROMS RESOLUTION
Authors : Reinemer, P.; Dirr, H.W.; Ladenstein, R.; Lobello, M.; Federici, G.; Huber, R.; Parker, M.W.
Deposited on : 1992-05-28
Resolution : 2.80 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)
Xtrriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

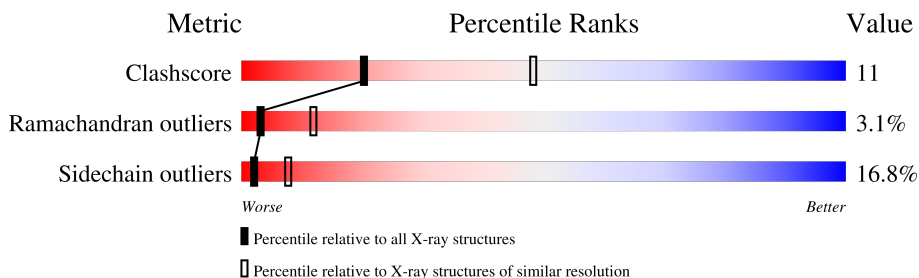
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	209	
1	B	209	

2 Entry composition [i](#)

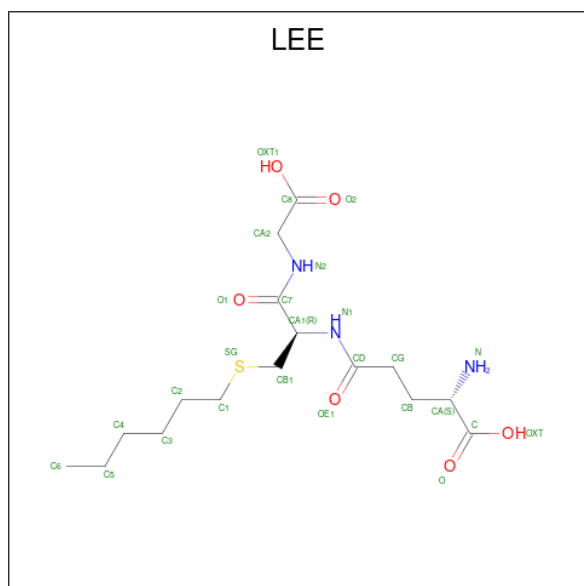
There are 3 unique types of molecules in this entry. The entry contains 3533 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUTATHIONE S-TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1638	1052	272	308	6			
1	B	209	Total	C	N	O	S	0	0	0
			1638	1052	272	308	6			

- Molecule 2 is L-gamma-glutamyl-S-hexyl-L-cysteinylglycine (CCD ID: LEE) (formula: $C_{16}H_{29}N_3O_6S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	16	3	6	1		
2	B	1	Total	C	N	O	S	0	0
			26	16	3	6	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	102	Total 102	O 102	0	0
3	B	103	Total 103	O 103	0	0

3 Residue-property plots

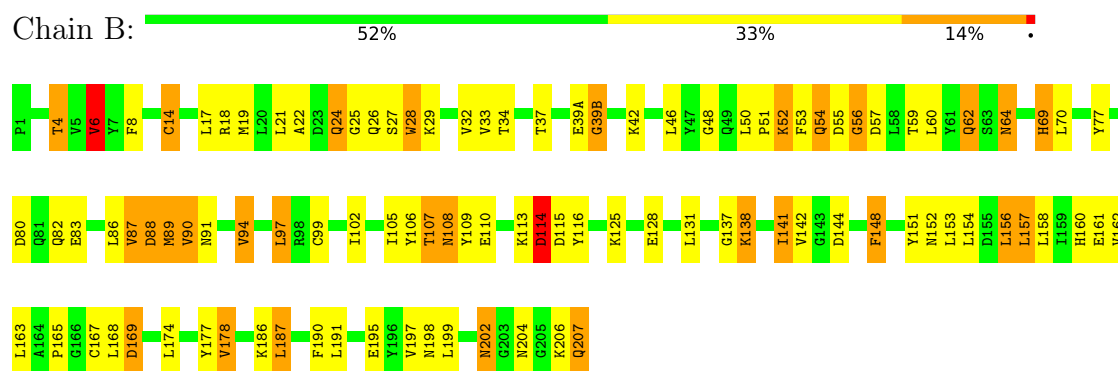
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: GLUTATHIONE S-TRANSFERASE



• Molecule 1: GLUTATHIONE S-TRANSFERASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	60.50Å 60.50Å 238.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	EREF, X-PLOR	Depositor
R, R_{free}	0.196 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3533	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LEE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.06	5/1673 (0.3%)	2.00	57/2269 (2.5%)
1	B	1.06	3/1673 (0.2%)	2.04	66/2269 (2.9%)
All	All	1.06	8/3346 (0.2%)	2.02	123/4538 (2.7%)

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	A	0	1
1	B	0	1
All	All	0	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	160	HIS	CD2-NE2	-7.34	1.29	1.37
1	B	6	VAL	CA-CB	7.17	1.63	1.54
1	B	69	HIS	CD2-NE2	-6.69	1.30	1.37
1	B	160	HIS	CD2-NE2	-6.52	1.30	1.37
1	A	141	ILE	CA-CB	6.12	1.62	1.54
1	A	69	HIS	CD2-NE2	-5.92	1.31	1.37
1	A	178	VAL	CA-CB	5.57	1.61	1.54
1	A	94	VAL	CA-CB	5.40	1.60	1.54

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	80	ASP	CA-CB-CG	11.96	124.56	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	HIS	CA-CB-CG	-11.20	102.61	113.80
1	B	202	ASN	OD1-CG-ND2	-10.64	111.96	122.60
1	A	81	GLN	OE1-CD-NE2	-10.10	112.50	122.60
1	A	108	ASN	CA-CB-CG	10.08	122.68	112.60
1	B	114	ASP	CA-CB-CG	9.07	121.67	112.60
1	B	207	GLN	OE1-CD-NE2	-8.60	114.00	122.60
1	B	56	GLY	N-CA-C	-7.69	94.95	113.18
1	B	202	ASN	CB-CG-ND2	7.67	127.91	116.40
1	B	55	ASP	CA-CB-CG	7.61	120.21	112.60
1	B	163	LEU	CB-CA-C	-7.48	97.96	110.68
1	A	66	ILE	N-CA-C	-7.43	103.44	110.42
1	B	138	LYS	CB-CG-CD	7.40	128.32	111.30
1	B	89	MET	CA-CB-CG	-7.29	99.53	114.10
1	A	171	PHE	CA-C-N	7.17	126.43	118.97
1	A	171	PHE	C-N-CA	7.17	126.43	118.97
1	A	195	GLU	CA-CB-CG	7.09	128.27	114.10
1	A	96	ASP	CA-CB-CG	7.05	119.66	112.60
1	A	57	ASP	N-CA-C	7.05	121.71	113.18
1	B	197	VAL	N-CA-C	7.04	117.80	110.62
1	A	202	ASN	N-CA-C	7.00	122.82	113.72
1	A	198	ASN	OD1-CG-ND2	-6.98	115.62	122.60
1	A	138	LYS	N-CA-C	-6.87	105.05	113.50
1	B	198	ASN	CA-CB-CG	6.84	119.44	112.60
1	B	152	ASN	OD1-CG-ND2	-6.81	115.79	122.60
1	B	107	THR	N-CA-CB	-6.81	100.65	110.80
1	B	39(A)	GLU	CB-CG-CD	6.76	124.09	112.60
1	B	107	THR	CA-CB-OG1	-6.70	99.55	109.60
1	B	86	LEU	CA-C-O	-6.66	113.36	120.42
1	A	59	THR	N-CA-C	-6.52	98.58	109.07
1	B	39(A)	GLU	CA-CB-CG	-6.51	101.08	114.10
1	A	81	GLN	CA-CB-CG	6.48	127.07	114.10
1	B	52	LYS	N-CA-C	-6.44	97.88	108.76
1	B	46	LEU	O-C-N	6.43	128.94	122.12
1	A	152	ASN	OD1-CG-ND2	-6.32	116.28	122.60
1	B	116	TYR	CA-C-O	-6.27	114.17	121.07
1	A	39	GLN	OE1-CD-NE2	-6.23	116.37	122.60
1	A	83	GLU	CA-CB-CG	6.19	126.47	114.10
1	A	134	ASN	CA-CB-CG	6.11	118.71	112.60
1	B	152	ASN	CA-CB-CG	6.02	118.62	112.60
1	B	199	LEU	N-CA-C	-6.02	99.89	109.04
1	A	14	CYS	CA-CB-SG	-6.01	100.58	114.40
1	B	160	HIS	CB-CG-CD2	-6.01	123.39	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	138	LYS	CG-CD-CE	5.98	125.06	111.30
1	A	1	PRO	CA-N-CD	-5.97	103.64	112.00
1	B	207	GLN	CG-CD-NE2	5.95	125.32	116.40
1	A	202	ASN	O-C-N	-5.93	115.06	122.35
1	B	14	CYS	O-C-N	-5.92	115.07	122.35
1	A	194	PRO	CA-CB-CG	-5.91	93.28	104.50
1	B	125	LYS	CA-C-N	5.87	125.34	119.24
1	B	125	LYS	C-N-CA	5.87	125.34	119.24
1	B	167	CYS	CA-C-O	5.86	126.76	120.20
1	B	50	LEU	O-C-N	-5.85	117.73	121.88
1	B	169	ASP	CA-CB-CG	-5.82	106.78	112.60
1	A	73	THR	N-CA-CB	-5.78	101.59	110.20
1	A	91	ASN	CA-CB-CG	-5.76	106.84	112.60
1	A	36	GLU	CB-CG-CD	5.73	122.34	112.60
1	A	69	HIS	CB-CG-CD2	-5.72	123.77	131.20
1	A	107	THR	CA-CB-OG1	-5.72	101.02	109.60
1	A	160	HIS	CB-CG-CD2	-5.70	123.80	131.20
1	B	51	PRO	N-CD-CG	-5.66	97.00	103.80
1	B	161	GLU	N-CA-C	-5.65	105.88	112.89
1	B	90	VAL	O-C-N	-5.64	116.03	121.90
1	B	28	TRP	CB-CG-CD1	-5.64	118.44	126.90
1	B	163	LEU	N-CA-CB	5.63	118.51	110.06
1	B	39(B)	GLY	CA-C-N	5.63	128.28	120.63
1	B	39(B)	GLY	C-N-CA	5.63	128.28	120.63
1	A	39(A)	GLU	CB-CG-CD	5.62	122.16	112.60
1	A	125	LYS	CA-C-O	-5.61	113.17	118.44
1	B	69	HIS	CB-CG-CD2	-5.58	123.95	131.20
1	B	87	VAL	N-CA-C	-5.57	104.13	111.09
1	A	53	PHE	CA-CB-CG	5.53	119.33	113.80
1	B	64	ASN	OD1-CG-ND2	5.52	128.12	122.60
1	A	131	LEU	O-C-N	-5.50	116.40	122.07
1	A	105	ILE	N-CA-C	5.49	116.26	110.72
1	B	148	PHE	N-CA-C	-5.48	106.43	113.01
1	B	167	CYS	N-CA-C	5.47	118.76	111.75
1	A	57	ASP	N-CA-CB	-5.46	101.24	110.41
1	B	108	ASN	CA-CB-CG	-5.46	107.14	112.60
1	A	86	LEU	CA-C-O	-5.46	114.64	120.42
1	B	52	LYS	CA-CB-CG	5.45	125.00	114.10
1	A	133	GLN	CA-CB-CG	5.44	124.98	114.10
1	A	133	GLN	OE1-CD-NE2	-5.43	117.17	122.60
1	A	139	THR	CA-C-O	5.43	123.53	119.68
1	A	152	ASN	CB-CG-ND2	5.42	124.53	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	THR	CA-C-N	5.36	127.26	120.72
1	A	65	THR	C-N-CA	5.36	127.26	120.72
1	A	48	GLY	O-C-N	-5.35	115.74	122.70
1	A	105	ILE	N-CA-CB	-5.34	102.58	110.58
1	B	128	GLU	CB-CG-CD	5.33	121.66	112.60
1	B	94	VAL	O-C-N	-5.33	116.70	121.87
1	B	107	THR	CA-CB-CG2	5.31	119.53	110.50
1	B	115	ASP	CA-CB-CG	5.29	117.89	112.60
1	B	28	TRP	CE2-CD2-CG	-5.26	100.89	107.20
1	A	30	GLU	CA-C-O	-5.25	114.96	120.58
1	A	180	ARG	O-C-N	-5.24	116.29	122.32
1	A	50	LEU	CA-C-O	-5.23	114.55	120.46
1	B	54	GLN	CA-CB-CG	-5.22	103.66	114.10
1	A	65	THR	CA-CB-OG1	-5.21	101.78	109.60
1	A	46	LEU	O-C-N	-5.21	116.60	122.12
1	B	162	VAL	CA-C-O	-5.20	115.28	121.05
1	B	64	ASN	CA-CB-CG	-5.18	107.42	112.60
1	A	180	ARG	CA-C-O	-5.15	114.33	120.56
1	A	207	GLN	OE1-CD-NE2	-5.14	117.46	122.60
1	A	24	GLN	N-CA-C	-5.14	106.86	112.72
1	A	58	LEU	CB-CA-C	-5.14	101.27	109.75
1	B	59	THR	CA-CB-OG1	-5.13	101.90	109.60
1	B	4	THR	CA-CB-OG1	-5.13	101.91	109.60
1	B	28	TRP	CG-CD2-CE3	5.13	139.03	133.90
1	A	1	PRO	N-CA-CB	5.13	108.64	103.00
1	A	51	PRO	N-CD-CG	-5.12	97.66	103.80
1	A	52	LYS	N-CA-C	-5.10	100.72	109.24
1	B	82	GLN	OE1-CD-NE2	-5.09	117.51	122.60
1	A	144	ASP	N-CA-C	5.09	117.72	111.82
1	B	152	ASN	CB-CG-ND2	5.08	124.02	116.40
1	B	24	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	B	178	VAL	CB-CA-C	-5.07	105.40	112.04
1	A	24	GLN	N-CA-CB	-5.05	103.17	110.70
1	B	62	GLN	OE1-CD-NE2	-5.03	117.57	122.60
1	B	57	ASP	CA-CB-CG	5.03	117.63	112.60
1	B	162	VAL	N-CA-C	-5.03	105.81	110.53
1	B	91	ASN	O-C-N	-5.02	116.80	122.12
1	B	207	GLN	CB-CG-CD	5.00	121.10	112.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	184	ARG	Peptide
1	B	77	TYR	Sidechain

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	1638	0	1643	43	0
1	B	1638	0	1643	34	0
2	A	26	0	27	1	0
2	B	26	0	27	0	0
3	A	102	0	0	3	0
3	B	103	0	0	2	0
All	All	3533	0	3340	75	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 11.

All (75) 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:105:ILE:HG21	1:B:202:ASN:HD22	1.57	0.68
1:A:87:VAL:HG12	1:A:142:VAL:HG11	1.77	0.66
1:B:14:CYS:O	1:B:18:ARG:HG3	1.95	0.66
1:A:4:THR:HG23	1:A:29:LYS:HB2	1.78	0.65
1:B:105:ILE:HG12	1:B:202:ASN:ND2	2.12	0.64
1:B:109:TYR:O	1:B:113:LYS:HB2	1.98	0.64
1:A:174:LEU:O	1:A:178:VAL:HG13	1.99	0.63
1:B:90:VAL:HG11	1:B:141:ILE:HG21	1.80	0.63
1:A:175:SER:O	1:A:178:VAL:HG22	2.01	0.61
1:B:97:LEU:HD12	1:B:156:LEU:HD21	1.85	0.58
1:B:105:ILE:HG21	1:B:202:ASN:ND2	2.20	0.57
1:A:157:LEU:HD22	1:A:168:LEU:HD11	1.87	0.56
1:B:153:LEU:HD23	1:B:177:TYR:CE2	2.41	0.56
1:A:21:LEU:HB3	1:A:26:GLN:HB2	1.86	0.56
1:A:6:VAL:HB	1:A:52:LYS:HB3	1.88	0.54
1:B:83:GLU:O	1:B:87:VAL:HG13	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:PHE:HA	1:B:33:VAL:O	2.08	0.54
1:B:19:MET:HE1	1:B:154:LEU:HD23	1.90	0.53
1:A:6:VAL:HG21	1:A:52:LYS:HD3	1.92	0.52
1:A:85:ALA:HB2	1:B:69:HIS:HD2	1.73	0.52
1:B:90:VAL:HG11	1:B:141:ILE:CG2	2.39	0.52
1:A:181:LEU:O	1:A:187:LEU:HD23	2.12	0.50
1:A:85:ALA:HB1	1:B:60:LEU:HD21	1.93	0.50
1:A:45:CYS:HA	1:A:61:TYR:CZ	2.47	0.49
1:A:54:GLN:HA	1:A:58:LEU:O	2.12	0.49
1:A:146:ILE:HD12	1:A:184:ARG:CZ	2.43	0.49
1:B:204:ASN:ND2	1:B:206:LYS:HG2	2.28	0.48
1:A:154:LEU:O	1:A:158:LEU:HG	2.14	0.48
1:B:19:MET:HB3	1:B:187:LEU:HD21	1.94	0.47
1:A:14:CYS:SG	1:A:51:PRO:HB3	2.56	0.46
1:B:190:PHE:HA	3:B:253:HOH:O	2.16	0.46
1:A:94:VAL:HG13	1:A:156:LEU:HD22	1.98	0.46
1:B:32:VAL:HG22	3:B:225:HOH:O	2.15	0.46
1:A:69:HIS:HA	1:A:72:ARG:NH1	2.31	0.46
1:B:53:PHE:CE2	1:B:70:LEU:HD11	2.51	0.46
1:A:128:GLU:HG3	1:A:173:LEU:HD22	1.98	0.45
1:A:184:ARG:NH1	3:A:293:HOH:O	2.48	0.45
1:A:3:TYR:HE1	1:A:55:ASP:OD1	1.99	0.45
1:B:24:GLN:O	1:B:26:GLN:N	2.49	0.45
1:B:157:LEU:HD23	1:B:178:VAL:CG2	2.46	0.45
1:A:204:ASN:HD21	1:A:206:LYS:HB2	1.82	0.45
1:A:90:VAL:HG22	1:A:130:LEU:HD13	1.99	0.45
1:B:148:PHE:HA	1:B:151:TYR:HD2	1.82	0.45
1:A:19:MET:HB3	1:A:187:LEU:HD11	1.99	0.44
1:A:170:ALA:O	1:A:172:PRO:HD3	2.17	0.44
1:B:87:VAL:HA	1:B:142:VAL:HG21	2.00	0.44
1:A:109:TYR:CG	1:A:206:LYS:HG2	2.53	0.44
1:B:6:VAL:HG22	1:B:52:LYS:HB3	1.99	0.44
1:B:22:ALA:HB2	1:B:28:TRP:HH2	1.82	0.44
1:A:87:VAL:HG13	1:A:142:VAL:HG21	2.00	0.44
1:B:94:VAL:HG22	1:B:153:LEU:HD12	2.00	0.44
1:A:15:ALA:O	1:A:19:MET:HG3	2.18	0.43
1:A:181:LEU:O	1:A:184:ARG:HG2	2.17	0.43
1:B:22:ALA:HB2	1:B:28:TRP:CH2	2.53	0.43
1:A:202:ASN:HB2	1:A:206:LYS:O	2.17	0.43
1:A:142:VAL:HG13	1:A:142:VAL:O	2.18	0.43
1:A:9:PRO:HD3	1:A:33:VAL:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:SER:O	1:A:107:THR:HB	2.19	0.43
1:B:4:THR:HB	1:B:54:GLN:HB2	2.00	0.42
1:A:139:THR:O	1:A:180:ARG:NH1	2.53	0.42
1:B:64:ASN:HD22	1:B:64:ASN:HA	1.52	0.42
1:A:9:PRO:HG3	1:A:32:VAL:CG1	2.49	0.42
2:A:208:LEE:HB31	3:A:263:HOH:O	2.19	0.42
1:A:81:GLN:HE21	1:A:81:GLN:HB3	1.71	0.42
1:A:188:LYS:HE3	1:A:188:LYS:HB3	1.83	0.42
1:A:86:LEU:O	1:A:90:VAL:HG23	2.20	0.41
1:A:120:LEU:HD11	1:A:160:HIS:HD2	1.85	0.41
1:A:68:ARG:HD2	1:B:88:ASP:OD2	2.19	0.41
1:B:131:LEU:HD12	1:B:137:GLY:HA2	2.01	0.41
1:A:80:ASP:OD1	1:A:83:GLU:HB2	2.21	0.41
1:B:105:ILE:HG22	1:B:106:TYR:CD2	2.56	0.41
1:B:202:ASN:OD1	1:B:202:ASN:N	2.55	0.40
1:B:42:LYS:HG3	1:B:48:GLY:O	2.22	0.40
1:A:156:LEU:O	1:A:159:ILE:HG12	2.21	0.40
1:A:102:ILE:HD12	3:A:310:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	207/209 (99%)	186 (90%)	15 (7%)	6 (3%)	3	13
1	B	207/209 (99%)	179 (86%)	21 (10%)	7 (3%)	3	11
All	All	414/418 (99%)	365 (88%)	36 (9%)	13 (3%)	3	12

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	25	GLY
1	A	142	VAL
1	B	108	ASN
1	A	195	GLU
1	B	114	ASP
1	B	165	PRO
1	A	62	GLN
1	A	204	ASN
1	A	63	SER
1	B	39(B)	GLY
1	B	62	GLN
1	A	194	PRO
1	B	56	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	176/176 (100%)	146 (83%)	30 (17%)	2	7
1	B	176/176 (100%)	147 (84%)	29 (16%)	2	8
All	All	352/352 (100%)	293 (83%)	59 (17%)	2	8

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	PRO
1	A	4	THR
1	A	17	LEU
1	A	40	SER
1	A	41	LEU
1	A	54	GLN
1	A	60	LEU
1	A	68	ARG
1	A	70	LEU
1	A	73	THR
1	A	81	GLN

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Mol	Chain	Res	Type
1	A	83	GLU
1	A	99	CYS
1	A	102	ILE
1	A	105	ILE
1	A	107	THR
1	A	113	LYS
1	A	115	ASP
1	A	118	LYS
1	A	121	PRO
1	A	132	SER
1	A	139	THR
1	A	146	ILE
1	A	147	SER
1	A	168	LEU
1	A	173	LEU
1	A	175	SER
1	A	194	PRO
1	A	199	LEU
1	A	206	LYS
1	B	6	VAL
1	B	17	LEU
1	B	21	LEU
1	B	27	SER
1	B	29	LYS
1	B	34	THR
1	B	37	THR
1	B	88	ASP
1	B	89	MET
1	B	97	LEU
1	B	99	CYS
1	B	102	ILE
1	B	107	THR
1	B	110	GLU
1	B	114	ASP
1	B	138	LYS
1	B	141	ILE
1	B	144	ASP
1	B	156	LEU
1	B	157	LEU
1	B	158	LEU
1	B	168	LEU
1	B	169	ASP

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Mol	Chain	Res	Type
1	B	174	LEU
1	B	186	LYS
1	B	187	LEU
1	B	191	LEU
1	B	195	GLU
1	B	207	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	81	GLN
1	A	82	GLN
1	A	135	GLN
1	A	145	GLN
1	B	24	GLN
1	B	54	GLN
1	B	64	ASN
1	B	69	HIS
1	B	91	ASN
1	B	152	ASN
1	B	202	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 ⓘ

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	LEE	B	208	-	24,25,25	1.61	2 (8%)	27,30,30	1.63	3 (11%)
2	LEE	A	208	-	24,25,25	0.94	1 (4%)	27,30,30	2.89	9 (33%)

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	LEE	B	208	-	-	5/30/30/30	-
2	LEE	A	208	-	-	10/30/30/30	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	208	LEE	OE1-CD	-6.61	1.10	1.23
2	B	208	LEE	OXT-C	-2.10	1.23	1.30
2	A	208	LEE	OXT1-C8	-2.06	1.24	1.30

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	208	LEE	CG-CD-N1	-7.20	103.19	115.86
2	A	208	LEE	OE1-CD-N1	6.16	133.38	122.95
2	A	208	LEE	CA1-C7-N2	5.51	128.37	116.54
2	A	208	LEE	CB1-CA1-N1	-4.59	99.04	111.06
2	A	208	LEE	O1-C7-N2	-4.51	113.45	122.98
2	A	208	LEE	CB1-CA1-C7	4.48	119.56	109.46
2	B	208	LEE	CG-CD-N1	-4.47	107.99	115.86
2	B	208	LEE	CB1-SG-C1	-3.97	90.48	102.26
2	A	208	LEE	CA1-CB1-SG	-3.48	100.28	113.92
2	A	208	LEE	CB-CG-CD	-3.46	105.34	113.06
2	B	208	LEE	CB-CG-CD	-2.04	108.50	113.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	208	LEE	C7-CA1-N1	-2.04	105.58	111.11

There are no chirality outliers.

All (15) torsion outliers are listed below:

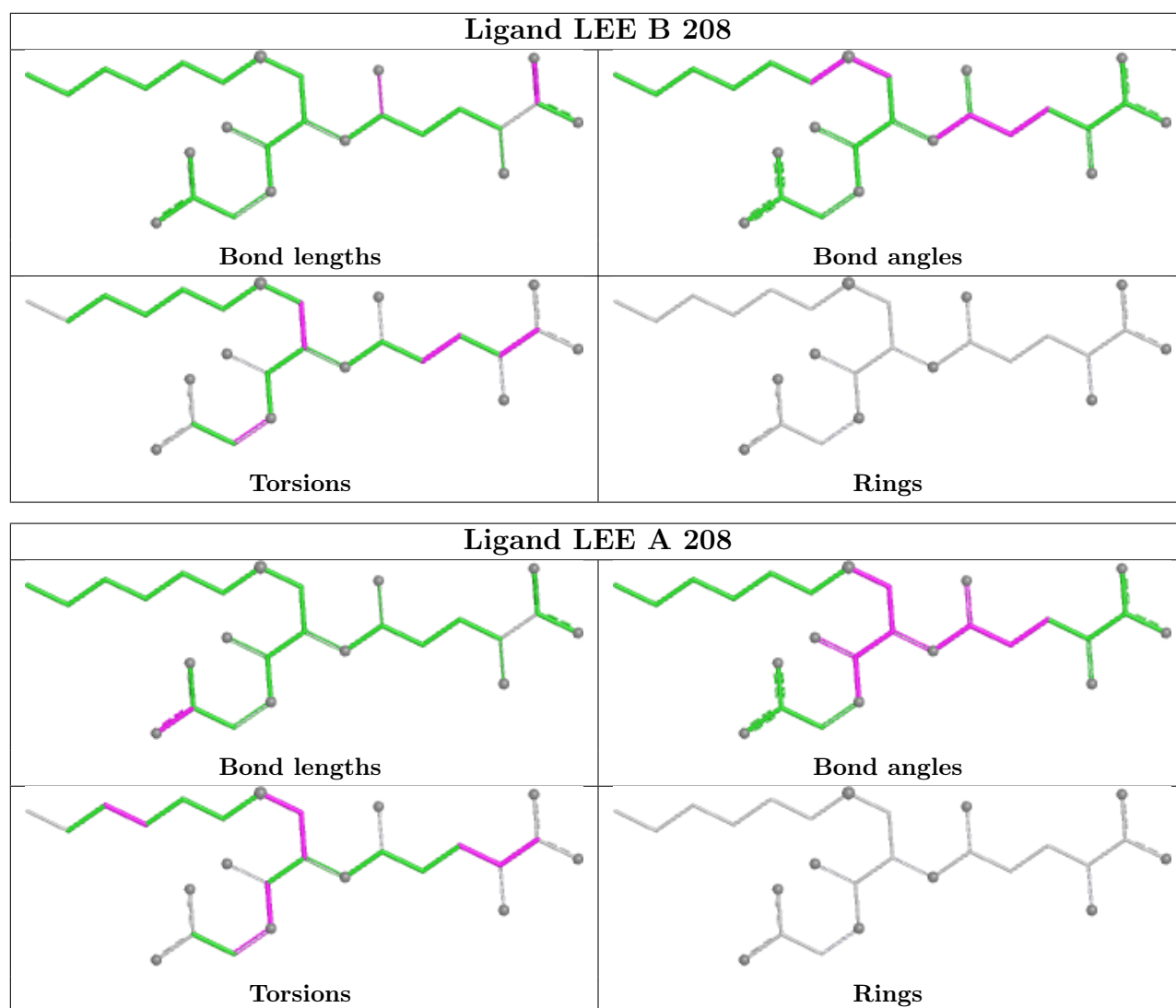
Mol	Chain	Res	Type	Atoms
2	A	208	LEE	O1-C7-N2-CA2
2	A	208	LEE	CA1-C7-N2-CA2
2	B	208	LEE	CA-CB-CG-CD
2	B	208	LEE	C7-CA1-CB1-SG
2	B	208	LEE	N1-CA1-CB1-SG
2	A	208	LEE	C2-C3-C4-C5
2	A	208	LEE	OXT-C-CA-CB
2	A	208	LEE	O-C-CA-CB
2	A	208	LEE	CA1-CB1-SG-C1
2	A	208	LEE	C7-CA1-CB1-SG
2	B	208	LEE	C8-CA2-N2-C7
2	A	208	LEE	C-CA-CB-CG
2	B	208	LEE	OXT-C-CA-N
2	A	208	LEE	N1-CA1-CB1-SG
2	A	208	LEE	C8-CA2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	208	LEE	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.