



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 28, 2024 – 05:33 PM EDT

PDB ID : 1R1S
Title : Structural Basis for Differential Recognition of Tyrosine Phosphorylated Sites in the Linker for Activation of T cells (LAT) by the Adaptor Protein Gads
Authors : Cho, S.; Mariuzza, R.A.
Deposited on : 2003-09-24
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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

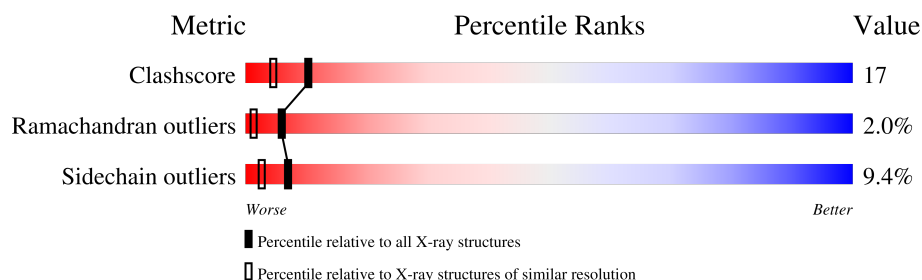
1 Overall quality at a glance

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))
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	100	61% 31% . .
1	C	100	53% 37% 5% . .
1	E	100	67% 19% 7% 6% .
1	G	100	60% 27% 9% .
2	B	7	14% 57% 29%
2	D	7	71% 29%
2	F	7	43% 29% 29%
2	H	7	57% 43%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4009 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 GRB2-related adaptor protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	96	Total	C	N	O	S	0	2	0
			808	518	139	149	2			
1	C	96	Total	C	N	O	S	0	0	0
			808	518	139	149	2			
1	E	99	Total	C	N	O	S	0	2	0
			839	540	144	153	2			
1	G	100	Total	C	N	O	S	0	2	0
			838	537	145	154	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	GLY	-	cloning artifact	UNP O89100
A	51	SER	-	cloning artifact	UNP O89100
C	50	GLY	-	cloning artifact	UNP O89100
C	51	SER	-	cloning artifact	UNP O89100
E	50	GLY	-	cloning artifact	UNP O89100
E	51	SER	-	cloning artifact	UNP O89100
G	50	GLY	-	cloning artifact	UNP O89100
G	51	SER	-	cloning artifact	UNP O89100

- Molecule 2 is a protein called LAT pY226 peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	7	Total	C	N	O	P	0	0	0
			60	35	7	17	1			
2	D	7	Total	C	N	O	P	0	0	0
			60	35	7	17	1			
2	F	7	Total	C	N	O	P	0	0	0
			60	35	7	17	1			
2	H	7	Total	C	N	O	P	0	0	0
			60	35	7	17	1			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	108	Total	O	0	0
			108	108		
4	B	15	Total	O	0	0
			15	15		
4	C	111	Total	O	0	0
			111	111		
4	D	8	Total	O	0	0
			8	8		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	92	Total 92	O 92	0	0
4	F	7	Total 7	O 7	0	0
4	G	88	Total 88	O 88	0	0
4	H	12	Total 12	O 12	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.

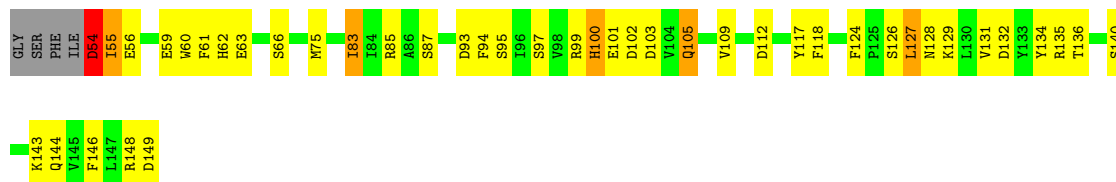
• Molecule 1: GRB2-related adaptor protein 2

Chain A: 



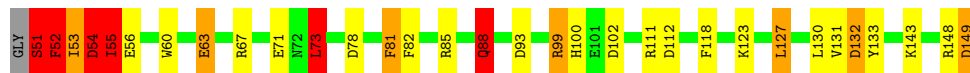
• Molecule 1: GRB2-related adaptor protein 2

Chain C: 



• Molecule 1: GRB2-related adaptor protein 2

Chain E: 




• Molecule 1: GRB2-related adaptor protein 2

Chain G: 



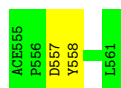
• Molecule 2: LAT pY226 peptide

Chain B: 



- Molecule 2: LAT pY226 peptide

Chain D:  71% 29%



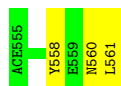
- Molecule 2: LAT pY226 peptide

Chain F:  43% 29% 29%



- Molecule 2: LAT pY226 peptide

Chain H:  57% 43%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.64Å 117.94Å 50.59Å 90.00° 108.92° 90.00°	Depositor
Resolution (Å)	30.00 – 1.90	Depositor
% Data completeness (in resolution range)	92.7 (30.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.213 , 0.259	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4009	wwPDB-VP
Average B, all atoms (Å ²)	36.0	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: ACE, PTR, SO4

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	1.77	14/830 (1.7%)	1.41	6/1115 (0.5%)
1	C	1.92	20/830 (2.4%)	1.68	15/1115 (1.3%)
1	E	1.59	7/867 (0.8%)	1.53	11/1165 (0.9%)
1	G	1.65	10/865 (1.2%)	1.48	15/1162 (1.3%)
2	B	1.83	0/41	2.31	3/53 (5.7%)
2	D	1.60	0/41	1.53	1/53 (1.9%)
2	F	2.21	2/41 (4.9%)	2.01	1/53 (1.9%)
2	H	1.57	0/41	1.43	0/53
All	All	1.74	53/3556 (1.5%)	1.54	52/4769 (1.1%)

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
1	E	0	1
1	G	0	2
All	All	0	4

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	559	GLU	CD-OE2	-9.35	1.15	1.25
1	C	85	ARG	CZ-NH2	9.08	1.44	1.33
1	C	134	TYR	CD2-CE2	-7.84	1.27	1.39
1	C	117	TYR	CE2-CZ	-7.77	1.28	1.38
1	C	109	VAL	CA-CB	-7.62	1.38	1.54
1	C	56	GLU	CD-OE1	7.35	1.33	1.25
1	G	138	SER	CB-OG	6.86	1.51	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	TYR	CD2-CE2	-6.85	1.29	1.39
1	E	133	TYR	CD2-CE2	-6.71	1.29	1.39
1	G	118	PHE	CE2-CZ	6.71	1.50	1.37
2	F	561	LEU	C-OXT	6.52	1.35	1.23
1	C	134	TYR	CD1-CE1	-6.41	1.29	1.39
1	G	52	PHE	CB-CG	-6.39	1.40	1.51
1	C	124	PHE	CD2-CE2	-6.31	1.26	1.39
1	E	55	ILE	CA-CB	6.17	1.69	1.54
1	C	105	GLN	CB-CG	-6.09	1.36	1.52
1	C	75	MET	CB-CG	5.87	1.70	1.51
1	E	88	GLN	CD-NE2	5.78	1.47	1.32
1	A	61	PHE	CE2-CZ	-5.77	1.26	1.37
1	A	133	TYR	CA-CB	-5.77	1.41	1.53
1	C	94	PHE	CG-CD1	5.77	1.47	1.38
1	C	59	GLU	CD-OE2	5.76	1.31	1.25
1	A	60	TRP	CB-CG	5.75	1.60	1.50
1	E	52	PHE	CA-C	5.72	1.67	1.52
1	A	59	GLU	C-O	5.72	1.34	1.23
1	C	127	LEU	C-O	5.70	1.34	1.23
1	A	97	SER	CB-OG	-5.70	1.34	1.42
1	A	117	TYR	CD1-CE1	5.60	1.47	1.39
1	E	51	SER	CB-OG	5.58	1.49	1.42
1	A	95	SER	C-O	-5.57	1.12	1.23
1	A	122	GLU	CD-OE2	-5.52	1.19	1.25
1	G	71	GLU	CD-OE2	-5.52	1.19	1.25
1	C	66	SER	CB-OG	-5.49	1.35	1.42
1	A	76	GLY	C-O	-5.45	1.15	1.23
1	A	137	THR	CA-CB	5.43	1.67	1.53
1	A	138	SER	CB-OG	-5.42	1.35	1.42
1	E	63	GLU	CD-OE1	-5.40	1.19	1.25
1	C	109	VAL	CB-CG2	5.39	1.64	1.52
1	G	87	SER	C-O	5.38	1.33	1.23
1	G	70	ALA	CA-CB	5.27	1.63	1.52
1	E	81	PHE	CE2-CZ	5.23	1.47	1.37
1	C	135	ARG	CZ-NH1	-5.22	1.26	1.33
1	G	66	SER	CB-OG	5.21	1.49	1.42
1	C	87	SER	CB-OG	5.17	1.49	1.42
1	G	146	PHE	CD1-CE1	5.17	1.49	1.39
1	C	54	ASP	N-CA	5.17	1.56	1.46
1	C	61	PHE	CE2-CZ	5.15	1.47	1.37
1	C	146	PHE	CE2-CZ	5.12	1.47	1.37
1	A	75	MET	SD-CE	5.10	2.06	1.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	56	GLU	CD-OE1	5.09	1.31	1.25
1	C	95	SER	C-O	-5.06	1.13	1.23
1	G	117	TYR	CB-CG	-5.03	1.44	1.51
1	A	85	ARG	CG-CD	-5.02	1.39	1.51

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	85	ARG	NE-CZ-NH1	-13.73	113.44	120.30
1	E	149	ASP	CB-CG-OD2	10.36	127.62	118.30
1	G	112	ASP	CB-CG-OD2	10.02	127.31	118.30
1	C	149	ASP	CB-CG-OD1	9.57	126.92	118.30
1	A	112	ASP	CB-CG-OD2	9.40	126.76	118.30
1	E	132	ASP	CB-CG-OD2	9.32	126.69	118.30
1	E	112	ASP	CB-CG-OD2	9.14	126.53	118.30
1	E	93	ASP	CB-CG-OD2	9.00	126.40	118.30
1	E	73	LEU	CB-CG-CD1	8.61	125.63	111.00
1	C	149	ASP	CB-CG-OD2	-8.47	110.68	118.30
1	G	85	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	C	102	ASP	CB-CG-OD2	8.22	125.70	118.30
1	G	78	ASP	CB-CG-OD2	8.21	125.69	118.30
1	C	112	ASP	CB-CG-OD2	8.20	125.68	118.30
1	A	78	ASP	CB-CG-OD1	-7.95	111.15	118.30
1	G	112	ASP	CB-CG-OD1	-7.72	111.35	118.30
1	G	148	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	E	52	PHE	CB-CA-C	7.42	125.24	110.40
2	F	557	ASP	CB-CG-OD2	7.20	124.78	118.30
1	C	85	ARG	NE-CZ-NH2	7.09	123.84	120.30
1	E	102	ASP	CB-CG-OD2	6.96	124.56	118.30
1	A	78	ASP	CB-CG-OD2	6.91	124.52	118.30
1	G	132	ASP	CB-CG-OD2	6.90	124.51	118.30
1	C	127	LEU	CB-CG-CD2	6.84	122.63	111.00
1	G	54	ASP	CB-CG-OD2	6.78	124.40	118.30
1	G	148	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	C	99	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	E	78[A]	ASP	CB-CG-OD2	6.46	124.11	118.30
1	C	93	ASP	CB-CG-OD2	6.39	124.05	118.30
1	E	85	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	A	112	ASP	CB-CG-OD1	-6.13	112.78	118.30
1	G	99	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	C	132	ASP	CB-CG-OD2	5.86	123.57	118.30
1	C	112	ASP	CB-CG-OD1	-5.67	113.20	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	55	ILE	N-CA-C	5.65	126.27	111.00
1	A	132	ASP	CB-CG-OD2	5.60	123.34	118.30
1	C	54	ASP	CB-CG-OD2	5.58	123.33	118.30
2	B	557	ASP	CB-CG-OD1	5.46	123.21	118.30
1	C	100	HIS	N-CA-C	-5.38	96.48	111.00
1	G	127	LEU	CB-CG-CD2	5.33	120.06	111.00
2	B	559	GLU	CB-CA-C	-5.29	99.81	110.40
1	E	85	ARG	NE-CZ-NH2	-5.29	117.65	120.30
1	A	133	TYR	CB-CA-C	-5.29	99.83	110.40
1	G	73	LEU	CB-CG-CD1	5.27	119.97	111.00
2	D	557	ASP	CB-CG-OD2	5.21	122.99	118.30
1	G	149	ASP	CB-CA-C	5.20	120.79	110.40
1	C	103	ASP	CB-CG-OD2	5.17	122.95	118.30
1	G	103	ASP	CB-CG-OD2	5.11	122.90	118.30
2	B	559	GLU	OE1-CD-OE2	5.10	129.42	123.30
1	E	130	LEU	CB-CG-CD1	-5.08	102.36	111.00
1	C	148	ARG	NE-CZ-NH1	-5.07	117.76	120.30
1	G	149	ASP	CB-CG-OD2	5.04	122.84	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	54	ASP	Peptide
1	E	55	ILE	Peptide
1	G	50	GLY	Peptide
1	G	51	SER	Peptide

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	808	0	771	37	0
1	C	808	0	775	21	0
1	E	839	0	801	46	0
1	G	838	0	799	29	0
2	B	60	0	44	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	60	0	44	0	0
2	F	60	0	44	2	0
2	H	60	0	44	2	0
3	A	10	0	0	1	0
3	C	10	0	0	1	0
3	E	10	0	0	1	0
3	G	5	0	0	1	0
4	A	108	0	0	8	0
4	B	15	0	0	0	0
4	C	111	0	0	3	0
4	D	8	0	0	0	0
4	E	92	0	0	2	0
4	F	7	0	0	0	0
4	G	88	0	0	2	0
4	H	12	0	0	0	0
All	All	4009	0	3322	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 17.

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:C:62:HIS:CE1	1:E:73:LEU:HD13	1.34	1.58
1:A:75:MET:SD	1:A:75:MET:CE	2.06	1.43
1:C:62:HIS:CE1	1:E:73:LEU:CD1	2.27	1.18
1:C:62:HIS:ND1	1:E:73:LEU:HD13	1.64	1.11
1:E:53:ILE:HG23	1:E:54:ASP:HA	1.11	1.07
1:E:51:SER:HB2	1:E:60:TRP:HB3	1.39	1.05
1:C:62:HIS:ND1	1:E:73:LEU:CD1	2.21	1.01
1:A:62:HIS:CE1	1:G:73:LEU:HD13	1.96	1.00
1:E:53:ILE:CG2	1:E:54:ASP:HA	1.96	0.95
1:A:93:ASP:OD1	1:A:108:LYS:NZ	2.04	0.91
1:E:51:SER:HB3	1:E:56:GLU:HG3	1.52	0.91
1:C:62:HIS:HE1	1:E:73:LEU:HD13	1.08	0.90
1:G:54:ASP:HA	1:G:55:ILE:HD12	1.58	0.84
1:E:53:ILE:HG23	1:E:54:ASP:CA	2.03	0.83
1:E:54:ASP:HB3	1:E:56:GLU:H	1.44	0.79
1:E:132:ASP:OD2	4:E:3558:HOH:O	2.01	0.78
1:E:127:LEU:O	1:E:127:LEU:HD23	1.84	0.77
1:A:56:GLU:OE2	1:C:55:ILE:HD12	1.85	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:3533:HOH:O	1:E:53:ILE:HD11	1.85	0.76
1:A:110:MET:HE1	2:B:561:LEU:HD13	1.69	0.75
1:E:54:ASP:H	1:E:55:ILE:HA	1.53	0.74
1:A:100:HIS:CD2	1:A:105:GLN:HG3	2.24	0.72
1:A:55:ILE:CG2	1:E:88:GLN:HB2	2.21	0.71
1:A:62:HIS:ND1	1:G:73:LEU:HD13	2.05	0.71
1:A:110:MET:CE	2:B:561:LEU:HD13	2.21	0.70
1:C:62:HIS:ND1	1:E:73:LEU:HD11	2.04	0.70
1:G:114:LYS:NZ	3:G:3482:SO4:O3	2.25	0.69
1:G:63:GLU:OE2	4:G:3541:HOH:O	2.11	0.68
1:C:83:ILE:C	1:C:83:ILE:HD13	2.16	0.67
1:E:54:ASP:OD1	1:E:54:ASP:C	2.34	0.66
1:E:51:SER:O	1:E:52:PHE:HB3	1.96	0.65
1:E:127:LEU:C	1:E:127:LEU:CD2	2.64	0.65
1:A:100:HIS:CD2	1:A:105:GLN:CG	2.80	0.65
1:A:62:HIS:HE1	1:G:73:LEU:HD13	1.58	0.65
1:C:54:ASP:HB2	4:C:3582:HOH:O	1.98	0.63
1:A:79:ILE:HG13	4:A:3564:HOH:O	1.98	0.63
1:A:79:ILE:O	1:A:148:ARG:HD3	2.00	0.62
1:E:54:ASP:OD1	1:E:54:ASP:O	2.18	0.61
1:A:121:THR:HB	3:A:3484:SO4:O4	2.00	0.61
1:A:55:ILE:HG21	1:E:88:GLN:HB2	1.82	0.59
1:A:120:TRP:CH2	2:B:560:ASN:HA	2.37	0.59
1:G:52:PHE:C	1:G:54:ASP:H	2.06	0.59
1:E:127:LEU:HD23	1:E:127:LEU:C	2.23	0.58
1:G:120:TRP:CH2	2:H:560:ASN:HA	2.39	0.58
1:A:101:GLU:N	4:A:3564:HOH:O	2.38	0.56
1:A:62:HIS:CE1	1:G:73:LEU:CD1	2.82	0.56
1:A:62:HIS:ND1	1:G:73:LEU:CD1	2.69	0.56
1:E:55:ILE:HG12	1:E:55:ILE:O	2.05	0.55
1:A:55:ILE:CG2	1:A:55:ILE:O	2.54	0.54
1:E:51:SER:HB2	1:E:60:TRP:CB	2.25	0.54
1:G:52:PHE:HB3	1:G:54:ASP:C	2.27	0.54
1:E:54:ASP:H	1:E:55:ILE:CA	2.20	0.53
1:E:54:ASP:CB	1:E:56:GLU:H	2.16	0.53
1:C:100:HIS:CD2	1:C:105:GLN:HG3	2.44	0.53
1:A:63:GLU:HG3	1:E:63:GLU:HG2	1.90	0.52
1:G:56:GLU:HA	4:G:3567:HOH:O	2.08	0.52
1:E:51:SER:HB3	1:E:56:GLU:CG	2.34	0.52
1:E:52:PHE:CD2	1:E:53:ILE:N	2.78	0.52
1:E:52:PHE:O	1:E:54:ASP:HB3	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:52:PHE:C	1:G:54:ASP:N	2.62	0.52
1:G:54:ASP:CA	1:G:55:ILE:HD12	2.36	0.52
1:G:51:SER:HB3	1:G:128:ASN:HB2	1.92	0.51
1:E:82:PHE:CE1	1:E:149:ASP:HB3	2.46	0.51
1:A:75:MET:CE	1:A:75:MET:CG	2.88	0.51
1:E:127:LEU:O	1:E:127:LEU:CD2	2.57	0.50
1:E:127:LEU:CD2	1:E:131:VAL:HG23	2.42	0.50
1:C:101:GLU:HB3	4:C:3558:HOH:O	2.11	0.50
1:C:83:ILE:HD13	1:C:83:ILE:O	2.12	0.50
1:A:56:GLU:HG3	4:A:3547:HOH:O	2.11	0.49
1:G:52:PHE:HB2	1:G:55:ILE:N	2.28	0.49
1:A:100:HIS:NE2	1:A:105:GLN:HG3	2.26	0.49
1:C:83:ILE:HD12	1:C:97:SER:HB2	1.94	0.49
1:C:100:HIS:NE2	1:C:105:GLN:HG3	2.28	0.49
1:A:100:HIS:CD2	1:A:105:GLN:HG2	2.48	0.48
1:A:144:GLN:HG3	4:A:3575:HOH:O	2.14	0.48
1:G:55:ILE:CG2	1:G:56:GLU:N	2.76	0.48
1:E:51:SER:N	4:E:3578:HOH:O	2.46	0.48
1:E:67:ARG:O	1:E:71:GLU:HG3	2.13	0.48
1:E:54:ASP:HB3	1:E:56:GLU:N	2.21	0.48
1:G:51:SER:O	1:G:128:ASN:ND2	2.48	0.47
1:E:81:PHE:HA	1:E:148:ARG:O	2.15	0.47
1:C:60:TRP:CH2	1:C:131:VAL:HG21	2.50	0.46
1:G:74:LEU:HB2	1:G:104:VAL:HG21	1.96	0.46
2:F:558:PTR:CE1	2:F:558:PTR:O2P	2.64	0.46
1:A:61:PHE:O	1:A:62:HIS:HD2	2.00	0.45
1:A:110:MET:HE1	2:B:561:LEU:CD1	2.44	0.45
1:C:62:HIS:O	1:C:63:GLU:C	2.55	0.45
1:E:53:ILE:N	1:E:54:ASP:HB2	2.32	0.45
1:G:52:PHE:CG	1:G:60:TRP:HA	2.51	0.45
2:F:561:LEU:HD12	2:F:561:LEU:HA	1.81	0.44
1:C:126:SER:OG	3:C:3487:SO4:O4	2.29	0.44
1:A:56:GLU:OE2	1:G:88:GLN:NE2	2.50	0.44
1:A:55:ILE:HG23	1:E:88:GLN:HB2	1.98	0.44
1:E:118:PHE:HB3	1:E:123:LYS:HG2	1.99	0.43
1:A:101:GLU:CA	4:A:3564:HOH:O	2.67	0.43
1:A:67:ARG:CZ	2:B:556:PRO:HB2	2.48	0.43
1:C:129:LYS:NZ	4:C:3545:HOH:O	2.51	0.43
1:G:54:ASP:N	1:G:55:ILE:HA	2.34	0.42
1:G:52:PHE:CB	1:G:55:ILE:N	2.82	0.42
1:A:110:MET:HE3	2:B:561:LEU:HD13	1.99	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:3541:HOH:O	1:E:111:ARG:HD3	2.20	0.42
1:E:99:ARG:HD2	1:E:100:HIS:O	2.20	0.42
1:C:118:PHE:HZ	1:G:113:THR:HG22	1.84	0.42
1:G:120:TRP:CZ3	2:H:560:ASN:HA	2.55	0.42
1:A:79:ILE:CG1	4:A:3564:HOH:O	2.61	0.42
1:E:53:ILE:CB	1:E:54:ASP:HA	2.49	0.42
1:G:55:ILE:HG23	1:G:56:GLU:HB2	2.02	0.41
1:A:100:HIS:NE2	1:A:105:GLN:CG	2.83	0.41
1:G:50:GLY:O	1:G:128:ASN:ND2	2.52	0.41
1:C:62:HIS:HE1	1:E:73:LEU:CD1	1.98	0.41
1:G:57:PHE:CD2	1:G:57:PHE:C	2.93	0.41
1:A:93:ASP:CB	1:A:108:LYS:NZ	2.84	0.41
1:E:55:ILE:O	1:E:55:ILE:CG1	2.64	0.41
1:A:113:THR:HG23	3:E:3483:SO4:O4	2.21	0.40
1:G:51:SER:HB3	1:G:128:ASN:CB	2.51	0.40
1:C:83:ILE:CD1	1:C:97:SER:HB2	2.50	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	94/100 (94%)	91 (97%)	3 (3%)	0	100	100
1	C	94/100 (94%)	89 (95%)	4 (4%)	1 (1%)	12	4
1	E	98/100 (98%)	90 (92%)	5 (5%)	3 (3%)	3	0
1	G	99/100 (99%)	93 (94%)	2 (2%)	4 (4%)	2	0
2	B	4/7 (57%)	4 (100%)	0	0	100	100
2	D	4/7 (57%)	4 (100%)	0	0	100	100
2	F	4/7 (57%)	4 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	4/7 (57%)	4 (100%)	0	0	100	100
All	All	401/428 (94%)	379 (94%)	14 (4%)	8 (2%)	6	1

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	55	ILE
1	E	53	ILE
1	G	54	ASP
1	E	52	PHE
1	E	54	ASP
1	G	51	SER
1	G	53	ILE
1	G	55	ILE

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	89/92 (97%)	86 (97%)	3 (3%)	32	25
1	C	89/92 (97%)	81 (91%)	8 (9%)	8	3
1	E	93/92 (101%)	84 (90%)	9 (10%)	6	2
1	G	92/92 (100%)	78 (85%)	14 (15%)	2	0
2	B	5/5 (100%)	3 (60%)	2 (40%)	0	0
2	D	5/5 (100%)	5 (100%)	0	100	100
2	F	5/5 (100%)	5 (100%)	0	100	100
2	H	5/5 (100%)	4 (80%)	1 (20%)	1	0
All	All	383/388 (99%)	346 (90%)	37 (10%)	7	2

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	GLU
1	A	114	LYS
1	A	122	GLU
2	B	557	ASP
2	B	561	LEU
1	C	54	ASP
1	C	83	ILE
1	C	127	LEU
1	C	128	ASN
1	C	136	THR
1	C	140	SER
1	C	143	LYS
1	C	144	GLN
1	E	51	SER
1	E	52	PHE
1	E	54	ASP
1	E	55	ILE
1	E	73	LEU
1	E	88	GLN
1	E	99	ARG
1	E	127	LEU
1	E	143	LYS
1	G	55	ILE
1	G	58	PRO
1	G	62[A]	HIS
1	G	62[B]	HIS
1	G	73	LEU
1	G	78	ASP
1	G	88	GLN
1	G	99	ARG
1	G	100	HIS
1	G	114	LYS
1	G	121	THR
1	G	127	LEU
1	G	143	LYS
1	G	148	ARG
2	H	561	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	105	GLN
1	C	142	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	68	HIS
1	E	88	GLN
1	E	142	GLN
1	G	68[A]	HIS
1	G	88	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	$\# Z > 2$
2	PTR	F	558	2	15,16,17	2.30	3 (20%)	17,22,24	1.75	6 (35%)
2	PTR	H	558	2	15,16,17	2.25	5 (33%)	17,22,24	1.46	3 (17%)
2	PTR	B	558	2	15,16,17	2.37	5 (33%)	17,22,24	1.15	2 (11%)
2	PTR	D	558	2	15,16,17	1.97	5 (33%)	17,22,24	1.46	3 (17%)

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	PTR	F	558	2	-	2/10/11/13	0/1/1/1
2	PTR	H	558	2	-	0/10/11/13	0/1/1/1
2	PTR	B	558	2	-	3/10/11/13	0/1/1/1
2	PTR	D	558	2	-	1/10/11/13	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	558	PTR	OH-CZ	-7.00	1.24	1.40
2	B	558	PTR	OH-CZ	-6.52	1.26	1.40
2	H	558	PTR	OH-CZ	-5.46	1.28	1.40
2	D	558	PTR	OH-CZ	-4.82	1.29	1.40
2	H	558	PTR	CE1-CD1	4.00	1.45	1.38
2	B	558	PTR	CD1-CG	3.53	1.45	1.38
2	H	558	PTR	CB-CG	3.03	1.58	1.51
2	H	558	PTR	CE2-CD2	3.02	1.43	1.38
2	B	558	PTR	P-O1P	2.79	1.59	1.50
2	D	558	PTR	CD1-CG	2.71	1.44	1.38
2	F	558	PTR	CB-CA	2.55	1.59	1.53
2	D	558	PTR	CE1-CD1	2.52	1.42	1.38
2	B	558	PTR	CE1-CZ	2.42	1.43	1.38
2	D	558	PTR	CE2-CD2	2.20	1.42	1.38
2	F	558	PTR	O-C	2.18	1.28	1.20
2	B	558	PTR	CE1-CD1	2.17	1.42	1.38
2	D	558	PTR	CD2-CG	-2.12	1.34	1.38
2	H	558	PTR	CE1-CZ	2.11	1.42	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	558	PTR	O3P-P-O1P	-3.51	97.15	110.83
2	F	558	PTR	OH-CZ-CE1	3.31	129.14	119.22
2	H	558	PTR	OH-CZ-CE1	2.94	128.02	119.22
2	F	558	PTR	OH-CZ-CE2	-2.75	110.97	119.22
2	F	558	PTR	OH-P-O1P	-2.73	100.36	109.48
2	F	558	PTR	O2P-P-OH	-2.52	97.86	105.32
2	F	558	PTR	O2P-P-O1P	2.49	120.52	110.83
2	B	558	PTR	OH-CZ-CE1	2.42	126.46	119.22
2	D	558	PTR	O2P-P-O1P	2.39	120.14	110.83
2	B	558	PTR	O2P-P-OH	2.33	112.21	105.32
2	H	558	PTR	O3P-P-O1P	2.24	119.57	110.83
2	F	558	PTR	O3P-P-OH	2.22	111.87	105.32
2	D	558	PTR	CE2-CZ-CE1	-2.20	116.95	120.16
2	H	558	PTR	O3P-P-O2P	-2.04	100.14	107.80

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	558	PTR	O-C-CA-CB

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	558	PTR	CZ-OH-P-O1P
2	F	558	PTR	CZ-OH-P-O1P
2	B	558	PTR	CZ-OH-P-O1P
2	B	558	PTR	CZ-OH-P-O3P
2	F	558	PTR	CZ-OH-P-O2P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	558	PTR	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	$\# Z > 2$
3	SO4	C	3485	-	4,4,4	1.35	0	6,6,6	1.35	1 (16%)
3	SO4	C	3487	-	4,4,4	0.82	0	6,6,6	1.23	1 (16%)
3	SO4	E	3483	-	4,4,4	0.41	0	6,6,6	0.88	0
3	SO4	A	3486	-	4,4,4	0.26	0	6,6,6	1.69	1 (16%)
3	SO4	A	3484	-	4,4,4	0.97	0	6,6,6	1.29	1 (16%)
3	SO4	G	3482	-	4,4,4	0.51	0	6,6,6	1.37	1 (16%)
3	SO4	E	3488	-	4,4,4	0.40	0	6,6,6	1.12	0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3485	SO4	O4-S-O2	2.51	122.70	109.56
3	G	3482	SO4	O4-S-O1	2.31	121.63	109.56
3	A	3486	SO4	O3-S-O2	2.30	121.58	109.56
3	A	3484	SO4	O3-S-O2	-2.17	98.23	109.56
3	C	3487	SO4	O3-S-O1	-2.03	98.97	109.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3487	SO4	1	0
3	E	3483	SO4	1	0
3	A	3484	SO4	1	0
3	G	3482	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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.