



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:00 AM UTC

PDB ID : 1FV1 / pdb_00001fv1
Title : STRUCTURAL BASIS FOR THE BINDING OF AN IMMUNODOMINANT PEPTIDE FROM MYELIN BASIC PROTEIN IN DIFFERENT REGISTERS BY TWO HLA-DR2 ALLELES
Authors : Li, H.; Mariuzza, A.R.; Li, Y.; Martin, R.
Deposited on : 2000-09-18
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

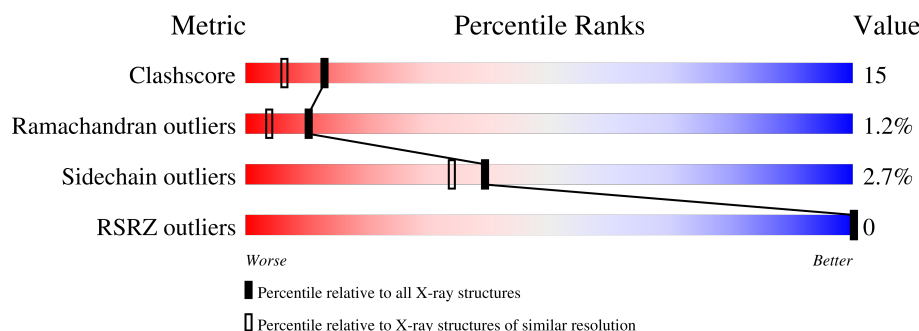
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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	181	70% 27% ..
1	D	181	65% 30% ..
2	B	190	67% 31% .
2	E	190	70% 29% .
3	C	20	50% 45% 5%
3	F	20	45% 40% 5% 10%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6795 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 MAJOR HISTOCOMPATIBILITY COMPLEX ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	179	Total	C	N	O	S	0	2	0
			1466	949	235	277	5			
1	D	178	Total	C	N	O	S	0	3	0
			1463	949	235	274	5			

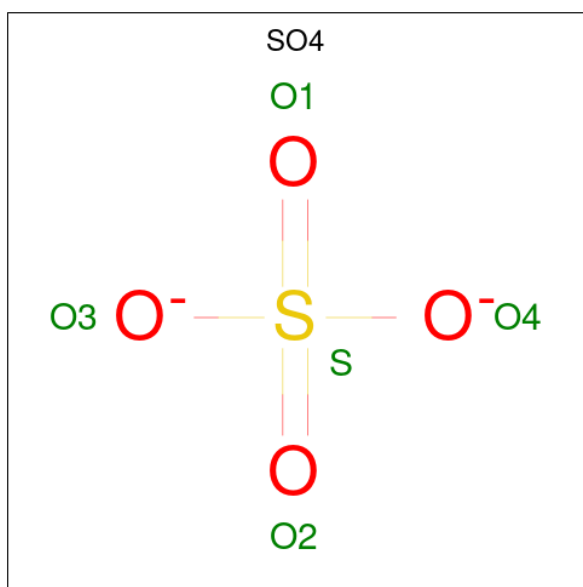
- Molecule 2 is a protein called MAJOR HISTOCOMPATIBILITY COMPLEX BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	190	Total	C	N	O	S	0	1	0
			1522	956	270	291	5			
2	E	190	Total	C	N	O	S	0	1	0
			1526	956	271	294	5			

- Molecule 3 is a protein called MYELIN BASIC PROTEIN.

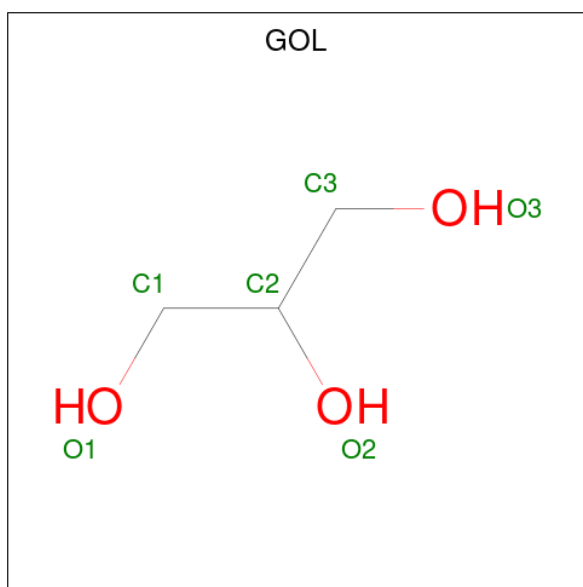
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	20	Total	C	N	O	0	0	0
			153	101	27	25			
3	F	18	Total	C	N	O	0	0	0
			144	97	25	22			

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	152	Total	O	0	0
			152	152		
6	B	86	Total	O	0	0
			86	86		
6	C	8	Total	O	0	0
			8	8		
6	D	148	Total	O	0	0
			148	148		
6	E	89	Total	O	0	0
			89	89		
6	F	11	Total	O	0	0
			11	11		

• Molecule 1: MAJOR HISTOCOMPATIBILITY COMPLEX ALPHA CHAIN

L1E	L122	L123	V132	F137	R140	L144	F145	R146	L151	T157	D162	C163	R164	V165	E166	H167	V169	G169	K176	H177	F180	D181	L1E	L1Y3	18	Q9	F12	P16	E21	D29	E30	I31	N36	T41	E47	F54	A59	N62	I63	E71	I72	M73	S77	T80	P81	V85	P86	P87	E88	V89	T90	V91	L92	P96	V97	E98	E101	I109	D110	K111	M118
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L1E	V119	L1F	V120	L1G	R123	L1H	T129	L1I	V132	L1J	V136	L1K	F137	L1L	V138	L1M	F139	L1N	R140	L1O	H143	L1P	F145	L1Q	R146	L1R	P155	L1S	S156	L1T	T157	L1U	Y161	L1V	D162	L1W	C163	L1X	R164	L1Y	V165	L1Z	E166	L2A	H167	L2B	V168	L2C	G169	L2D	L170	L2E	L174	L2F	L175	L2G	K176	L2H	H177	L2I	F180	L2J	D181	L2K	V182	L2L	V183	L2M	V184	L2N	V185	L2O	V186	L2P	V187	L2Q	V188	L2R	V189	L2S	V190	L2T	V191	L2U	V192	L2V	V193	L2W	V194	L2X	V195	L2Y	V196	L2Z	V197	L3A	V198	L3B	V199	L3C	V200	L3D	V201	L3E	V202	L3F	V203	L3G	V204	L3H	V205	L3I	V206	L3J	V207	L3K	V208	L3L	V209	L3M	V210	L3N	V211	L3O	V212	L3P	V213	L3Q	V214	L3R	V215	L3S	V216	L3T	V217	L3U	V218	L3V	V219	L3W	V220	L3X	V221	L3Y	V222	L3Z	V223	L4A	V224	L4B	V225	L4C	V226	L4D	V227	L4E	V228	L4F	V229	L4G	V230	L4H	V231	L4I	V232	L4J	V233	L4K	V234	L4L	V235	L4M	V236	L4N	V237	L4O	V238	L4P	V239	L4Q	V240	L4R	V241	L4S	V242	L4T	V243	L4U	V244	L4V	V245	L4W	V246	L4X	V247	L4Y	V248	L4Z	V249	L5A	V250	L5B	V251	L5C	V252	L5D	V253	L5E	V254	L5F	V255	L5G	V256	L5H	V257	L5I	V258	L5J	V259	L5K	V260	L5L	V261	L5M	V262	L5N	V263	L5O	V264	L5P	V265	L5Q	V266	L5R	V267	L5S	V268	L5T	V269	L5U	V270	L5V	V271	L5W	V272	L5X	V273	L5Y	V274	L5Z	V275	L6A	V276	L6B	V277	L6C	V278	L6D	V279	L6E	V280	L6F	V281	L6G	V282	L6H	V283	L6I	V284	L6J	V285	L6K	V286	L6L	V287	L6M	V288	L6N	V289	L6O	V290	L6P	V291	L6Q	V292	L6R	V293	L6S	V294	L6T	V295	L6U	V296	L6V	V297	L6W	V298	L6X	V299	L6Y	V300	L6Z	V301	L7A	V302	L7B	V303	L7C	V304	L7D	V305	L7E	V306	L7F	V307	L7G	V308	L7H	V309	L7I	V310	L7J	V311	L7K	V312	L7L	V313	L7M	V314	L7N	V315	L7O	V316	L7P	V317	L7Q	V318	L7R	V319	L7S	V320	L7T	V321	L7U	V322	L7V	V323	L7W	V324	L7X	V325	L7Y	V326	L7Z	V327	L8A	V328	L8B	V329	L8C	V330	L8D	V331	L8E	V332	L8F	V333	L8G	V334	L8H	V335	L8I	V336	L8J	V337	L8K	V338	L8L	V339	L8M	V340	L8N	V341	L8O	V342	L8P	V343	L8Q	V344	L8R	V345	L8S	V346	L8T	V347	L8U	V348	L8V	V349	L8W	V350	L8X	V351	L8Y	V352	L8Z	V353	L9A	V354	L9B	V355	L9C	V356	L9D	V357	L9E	V358	L9F	V359	L9G	V360	L9H	V361	L9I	V362	L9J	V363	L9K	V364	L9L	V365	L9M	V366	L9N	V367	L9O	V368	L9P	V369	L9Q	V370	L9R	V371	L9S	V372	L9T	V373	L9U	V374	L9V	V375	L9W	V376	L9X	V377	L9Y	V378	L9Z	V379	L0A	V380	L0B	V381	L0C	V382	L0D	V383	L0E	V384	L0F	V385	L0G	V386	L0H	V387	L0I	V388	L0J	V389	L0K	V390	L0L	V391	L0M	V392	L0N	V393	L0O	V394	L0P	V395	L0Q	V396	L0R	V397	L0S	V398	L0T	V399	L0U	V400	L0V	V401	L0W	V402	L0X	V403	L0Y	V404	L0Z	V405	L1A	V406	L1B	V407	L1C	V408	L1D	V409	L1E	V410	L1F	V411	L1G	V412	L1H	V413	L1I	V414	L1J	V415	L1K	V416	L1L	V417	L1M	V418	L1N	V419	L1O	V420	L1P	V421	L1Q
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R6	R9	Q10	R11	K12	Y13	L27	R28	R29	D30	I31	E36	L36	R39	D40	D41	E46	Y47	V50	T51	E52	L53	G54	R55	P56	Y60	M61	M62	D66	R71	V75	C79	R80	H81	E86	P97	K98	V99	T100	R105	T106	Q107	T108	L109	C110
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● Molecule 3: MYELIN BASIC PROTEIN



● Molecule 3: MYELIN BASIC PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.19Å 114.89Å 63.17Å 90.00° 90.90° 90.00°	Depositor
Resolution (Å)	100.00 – 1.90 63.18 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (100.00-1.90) 90.6 (63.18-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.31 (at 1.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.233 , 0.267 0.243 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.7	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.035 for -l,k,h 0.044 for -h,-k,l 0.467 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6795	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.92% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.47	0/1519	0.95	7/2073 (0.3%)
1	D	0.41	0/1520	0.92	7/2074 (0.3%)
2	B	0.37	0/1565	0.90	4/2131 (0.2%)
2	E	0.36	0/1569	0.89	3/2132 (0.1%)
3	C	0.49	0/160	1.06	1/219 (0.5%)
3	F	0.50	0/151	1.09	1/208 (0.5%)
All	All	0.41	0/6484	0.92	23/8837 (0.3%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	120	ASN	N-CA-C	7.39	121.54	109.72
2	B	110	GLN	N-CA-C	7.11	118.56	108.54
3	C	92	PHE	N-CA-C	-6.60	100.71	110.48
3	F	92	PHE	N-CA-C	-6.59	100.72	110.48
2	B	120	ASN	N-CA-C	6.48	120.26	109.95
2	E	110	GLN	N-CA-C	6.34	117.48	108.54
2	B	108	THR	N-CA-C	-6.12	98.92	108.90
1	D	163	CYS	N-CA-C	-6.06	98.64	108.52
1	A	88	GLU	N-CA-C	-6.03	99.42	109.24
2	E	79	CYS	N-CA-C	5.97	117.48	110.97
1	A	144	LEU	N-CA-C	-5.96	100.62	109.86
1	A	85	VAL	CA-C-N	5.90	123.97	119.66
1	A	85	VAL	C-N-CA	5.90	123.97	119.66
1	D	144	LEU	N-CA-C	-5.84	100.81	109.86
2	B	79	CYS	N-CA-C	5.64	117.11	110.97
1	D	31	ILE	N-CA-C	-5.58	105.41	110.82
1	A	163	CYS	N-CA-C	-5.56	99.45	108.52
1	D	110	ASP	N-CA-C	5.56	118.14	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	31	ILE	N-CA-C	-5.44	105.55	110.82
1	D	88	GLU	N-CA-C	-5.35	100.52	109.24
1	A	110	ASP	N-CA-C	5.23	117.63	109.52
1	D	85	VAL	CA-C-N	5.18	123.44	119.66
1	D	85	VAL	C-N-CA	5.18	123.44	119.66

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1466	0	1379	44	0
1	D	1463	0	1393	53	0
2	B	1522	0	1393	57	0
2	E	1526	0	1400	49	0
3	C	153	0	150	9	0
3	F	144	0	149	7	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	D	5	0	0	1	0
5	B	6	0	8	2	0
5	D	6	0	8	1	0
6	A	152	0	0	4	0
6	B	86	0	0	0	0
6	C	8	0	0	0	0
6	D	148	0	0	4	0
6	E	89	0	0	4	0
6	F	11	0	0	0	0
All	All	6795	0	5880	183	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 15.

All (183) 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)
2:B:107:GLN:HE22	2:B:114:LEU:HB3	1.24	0.98
1:D:14:LEU:HD11	2:E:6:ARG:HG3	1.46	0.97
2:E:13:TYR:OH	3:F:97:THR:HG22	1.74	0.86
1:A:73:MET:HE1	2:B:53:LEU:HG	1.56	0.85
2:B:13:TYR:OH	3:C:97:THR:HG22	1.79	0.82
1:A:36:MET:CE	1:A:63:ILE:HG13	2.13	0.79
1:D:93[B]:THR:HG22	1:D:95:SER:H	1.48	0.76
2:B:104:ALA:HB3	2:B:107:GLN:HE21	1.52	0.74
2:B:94[A]:ARG:HG3	2:B:94[A]:ARG:HH11	1.52	0.74
2:B:104:ALA:HB3	2:B:107:GLN:NE2	2.02	0.74
1:D:164:ARG:HH12	1:D:166:GLU:CD	1.95	0.73
2:E:115:LEU:HD21	2:E:188:TRP:CE3	2.24	0.72
2:E:98:LYS:HE3	2:E:100:THR:HG23	1.70	0.72
1:D:140:ARG:HH12	5:D:183:GOL:H11	1.53	0.72
1:A:181:ASP:HA	2:B:105:ARG:HH22	1.54	0.72
2:E:116:VAL:HG22	2:E:160:MET:HG3	1.73	0.70
1:D:17:ASP:OD1	2:E:6:ARG:HD2	1.92	0.69
1:D:167:HIS:HD2	1:D:169:GLY:H	1.39	0.68
2:B:170:VAL:HG23	2:B:170:VAL:O	1.92	0.68
1:A:36:MET:HE1	1:A:63:ILE:HG13	1.73	0.68
1:D:16:PRO:HD2	2:E:6:ARG:HD3	1.76	0.68
1:D:167:HIS:CD2	1:D:169:GLY:H	2.12	0.68
1:A:167:HIS:HD2	1:A:169:GLY:H	1.43	0.67
1:A:181:ASP:HA	2:B:105:ARG:NH2	2.09	0.67
2:B:105:ARG:NH2	2:B:105:ARG:HB3	2.09	0.66
2:B:35:GLU:OE1	2:E:52:GLU:HG3	1.95	0.66
1:A:110:ASP:OD1	1:A:146:ARG:HG2	1.96	0.66
1:A:41:THR:HG21	1:A:54:PHE:O	1.96	0.65
1:A:36:MET:HE2	1:A:63:ILE:HG13	1.78	0.64
1:D:62:ASN:ND2	3:F:97:THR:HG23	2.12	0.64
1:D:101:GLU:HG2	6:D:270:HOH:O	1.96	0.64
2:B:134:ASN:ND2	2:B:170:VAL:HG22	2.12	0.64
1:D:181:ASP:C	2:E:105:ARG:HH22	2.05	0.64
1:A:167:HIS:CD2	1:A:169:GLY:H	2.15	0.64
2:E:98:LYS:HE3	2:E:100:THR:CG2	2.28	0.63
2:B:2:ASP:CG	2:B:6:ARG:HH22	2.06	0.62
1:D:36:MET:CE	1:D:63:ILE:HG13	2.29	0.62
1:D:181:ASP:C	2:E:105:ARG:NH2	2.58	0.62
1:D:123:ARG:HG3	1:D:161:TYR:CE2	2.35	0.61
1:A:47:GLU:HG3	6:A:280:HOH:O	1.99	0.61
1:D:50:ARG:HD2	6:D:298:HOH:O	2.00	0.60
1:A:73:MET:CE	2:B:53:LEU:HG	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:55:ARG:HB3	2:E:56:PRO:HD3	1.84	0.58
2:B:55:ARG:O	2:B:59:GLU:HG3	2.04	0.58
2:B:94[A]:ARG:HG3	2:B:94[A]:ARG:NH1	2.18	0.58
2:B:131:TRP:O	2:B:137:GLU:HA	2.03	0.58
1:D:136:VAL:O	1:D:138:LEU:HD22	2.04	0.57
1:A:77:SER:O	1:A:80:THR:HG22	2.05	0.57
1:A:111:LYS:HG2	1:A:140:ARG:CZ	2.34	0.57
1:D:14:LEU:HD11	2:E:6:ARG:CG	2.30	0.57
2:B:107:GLN:NE2	2:B:114:LEU:HB3	2.08	0.57
2:E:131:TRP:O	2:E:137:GLU:HA	2.05	0.56
1:D:4:GLU:HG2	1:D:5:HIS:CD2	2.40	0.56
1:A:164:ARG:HH12	1:A:166:GLU:CD	2.13	0.56
1:D:36:MET:HE2	1:D:63:ILE:HG21	1.88	0.56
1:A:90:THR:HG23	6:A:211:HOH:O	2.06	0.55
2:B:55:ARG:HB3	2:B:56:PRO:HD3	1.89	0.55
1:D:138:LEU:HD22	1:D:138:LEU:N	2.22	0.55
1:A:132:VAL:HG12	1:A:151:LEU:HD13	1.89	0.55
2:E:27:LEU:HD12	2:E:41:ASP:HA	1.89	0.54
2:E:114:LEU:HD11	2:E:160:MET:HB3	1.88	0.54
1:D:17:ASP:OD1	2:E:6:ARG:CD	2.56	0.54
1:D:73:MET:HE1	2:E:53:LEU:HB3	1.90	0.54
2:E:75:VAL:HG13	6:E:216:HOH:O	2.07	0.54
3:C:103:PRO:O	3:C:104:SER:HB3	2.08	0.54
2:E:36:GLU:HG2	2:E:50:VAL:HG11	1.89	0.54
2:E:132:PHE:CE2	2:E:137:GLU:HB2	2.44	0.53
1:A:162:ASP:OD1	1:A:177:HIS:ND1	2.42	0.53
1:A:3:GLU:HA	2:B:18:PHE:CE2	2.44	0.53
1:D:46:GLU:HG2	6:D:298:HOH:O	2.07	0.53
2:B:94[A]:ARG:HD3	5:B:192:GOL:H11	1.90	0.53
1:D:108:PHE:CE1	1:D:146:ARG:HG3	2.43	0.53
1:A:118:ASN:HB3	1:A:166:GLU:HB2	1.89	0.53
2:B:149:GLN:HG2	2:B:155:PHE:CE2	2.44	0.52
2:B:27:LEU:HD12	2:B:41:ASP:HA	1.92	0.52
2:B:108:THR:O	2:B:109:LEU:CB	2.58	0.51
1:A:98:GLU:CG	1:A:101[B]:GLU:CD	2.84	0.51
1:D:70:LEU:HD13	2:E:9:GLN:HB2	1.91	0.51
2:E:60:TYR:CE2	3:F:101:PRO:HG2	2.45	0.51
1:A:9:GLN:HB3	2:B:13:TYR:HB2	1.93	0.51
2:E:27:LEU:HD11	2:E:39:ARG:HD3	1.92	0.51
2:B:26:PHE:HB3	2:B:42:SER:HB3	1.92	0.50
1:A:3:GLU:HA	2:B:18:PHE:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93[B]:THR:CG2	1:D:95:SER:O	2.59	0.50
2:B:161:LEU:HD13	2:B:163:THR:CG2	2.42	0.50
2:E:142:VAL:HG22	2:E:161:LEU:HD13	1.94	0.50
1:D:180:PHE:CE1	2:E:105:ARG:NH2	2.80	0.50
1:A:181:ASP:CA	2:B:105:ARG:NH2	2.75	0.50
1:D:111:LYS:HG2	1:D:140:ARG:CZ	2.42	0.49
2:B:177:HIS:CG	2:B:178:PRO:HD2	2.47	0.49
6:A:288:HOH:O	3:C:103:PRO:HG3	2.13	0.49
1:D:129:THR:O	1:D:132:VAL:HG22	2.13	0.49
1:A:97:VAL:HG12	1:A:98:GLU:N	2.28	0.48
1:A:62:ASN:ND2	3:C:97:THR:HG23	2.28	0.48
1:D:36:MET:HE1	1:D:63:ILE:HG13	1.95	0.48
2:E:10:GLN:HB2	2:E:31:ILE:HB	1.94	0.48
2:E:117:CYS:HB2	2:E:131:TRP:CZ2	2.48	0.48
2:E:37:ASP:C	2:E:50:VAL:HG12	2.37	0.48
2:E:177:HIS:CD2	2:E:178:PRO:HD2	2.49	0.48
1:A:81:PRO:HB3	2:B:5:PRO:HB3	1.95	0.48
2:B:113:ASN:N	2:B:163:THR:O	2.46	0.48
2:B:60:TYR:CE2	3:C:101:PRO:HG2	2.49	0.48
2:B:13:TYR:CE2	3:C:95:ILE:HG21	2.49	0.48
2:E:177:HIS:CG	2:E:178:PRO:HD2	2.48	0.48
1:A:157:THR:HG22	1:A:180:PHE:CD1	2.48	0.48
1:D:162:ASP:OD1	1:D:177:HIS:ND1	2.46	0.48
1:A:92:LEU:HD23	1:A:92:LEU:N	2.29	0.47
1:D:9:GLN:HB3	2:E:13:TYR:HB2	1.96	0.47
2:B:176:GLU:HG2	2:B:183:PRO:HB3	1.95	0.47
1:A:21:GLU:OE2	1:A:137:PHE:O	2.32	0.47
1:D:108:PHE:HE1	1:D:146:ARG:HG3	1.78	0.47
2:E:119:VAL:HG21	2:E:129:VAL:HG21	1.97	0.47
2:B:105:ARG:HB3	2:B:105:ARG:CZ	2.44	0.47
1:D:93[B]:THR:HG21	1:D:95:SER:O	2.14	0.47
1:A:97:VAL:CG1	1:A:98:GLU:N	2.78	0.47
1:D:12:PHE:C	1:D:12:PHE:CD1	2.93	0.47
2:B:133:ARG:O	2:B:134:ASN:HB2	2.14	0.46
2:E:141:GLY:O	2:E:161:LEU:HD12	2.16	0.46
1:A:96:PRO:HD3	2:B:120:ASN:ND2	2.30	0.46
2:B:81:HIS:CD2	3:C:93:LYS:HG2	2.50	0.46
3:C:87:PRO:O	3:C:88:VAL:HB	2.15	0.46
3:C:86:ASN:N	3:C:87:PRO:HD3	2.31	0.46
2:B:117:CYS:HB2	2:B:131:TRP:CZ2	2.51	0.45
1:D:36:MET:HE2	1:D:63:ILE:HG13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:VAL:HG12	1:D:176:LYS:HG3	1.98	0.45
1:A:89:VAL:HG12	1:A:176:LYS:HG3	1.98	0.45
2:B:27:LEU:HD11	2:B:39:ARG:HD3	1.99	0.45
1:D:92:LEU:HD12	1:D:92:LEU:N	2.32	0.45
3:F:87:PRO:O	3:F:88:VAL:HB	2.17	0.45
1:D:157:THR:HG22	1:D:180:PHE:CD1	2.52	0.44
1:A:12:PHE:C	1:A:12:PHE:CD1	2.94	0.44
1:D:26:PHE:HB2	1:D:31:ILE:HD11	2.00	0.44
1:A:29:ASP:HB3	2:B:153:TRP:CE2	2.53	0.44
2:B:2:ASP:OD2	2:B:6:ARG:NH2	2.48	0.44
1:A:87:PRO:HB2	1:A:109:ILE:HG23	2.00	0.44
1:A:8:ILE:HG12	2:B:14:GLU:HG2	1.99	0.43
1:D:113:THR:OG1	1:D:114:PRO:HA	2.18	0.43
2:E:113:ASN:HD22	2:E:114:LEU:N	2.17	0.43
1:D:92:LEU:HD13	1:D:106:ILE:HB	2.00	0.43
1:D:167:HIS:HB3	1:D:170:LEU:HD22	2.01	0.43
1:D:164:ARG:NH1	1:D:166:GLU:CD	2.71	0.43
2:B:94[B]:ARG:HD3	5:B:192:GOL:H11	1.98	0.43
2:E:13:TYR:CE2	3:F:95:ILE:HG21	2.54	0.43
2:B:10:GLN:HB2	2:B:31:ILE:HB	2.00	0.43
1:D:123:ARG:HD2	4:D:182:SO4:O4	2.18	0.43
2:B:97:PRO:HB3	2:B:119:VAL:HG12	2.01	0.43
2:E:96:GLU:HA	2:E:97:PRO:HD3	1.87	0.43
1:A:16:PRO:HD2	2:B:6:ARG:HD3	2.01	0.42
1:A:122:LEU:HB2	1:A:162:ASP:HB2	2.01	0.42
2:B:60:TYR:O	2:B:64:GLN:HG2	2.18	0.42
1:A:123:ARG:NH2	6:A:214:HOH:O	2.53	0.42
1:D:90:THR:HG23	6:D:213:HOH:O	2.17	0.42
1:D:109:ILE:HD12	1:D:109:ILE:N	2.35	0.42
1:A:77:SER:O	1:A:80:THR:CG2	2.68	0.42
2:B:47:TYR:O	2:B:48:ARG:HG2	2.19	0.42
2:B:157:THR:C	2:B:158:LEU:HD12	2.44	0.42
1:D:118:ASN:HB3	1:D:166:GLU:HB2	2.01	0.42
1:D:143:HIS:HD2	2:E:12:LYS:NZ	2.17	0.42
2:B:94[A]:ARG:NH1	2:B:94[A]:ARG:CG	2.83	0.42
3:F:103:PRO:O	3:F:104:SER:HB3	2.19	0.42
2:E:36:GLU:O	2:E:50:VAL:HG13	2.19	0.42
1:A:109:ILE:HD12	1:A:109:ILE:N	2.34	0.42
2:B:107:GLN:HE22	2:B:114:LEU:CB	2.12	0.42
1:D:99:LEU:HA	1:D:155:PRO:HB2	2.01	0.42
1:D:120:THR:HB	1:D:164:ARG:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:GLU:CD	1:D:47:GLU:H	2.27	0.42
2:E:29:ARG:HG2	2:E:36:GLU:OE2	2.20	0.42
2:E:189:ARG:CB	6:E:267:HOH:O	2.67	0.42
2:B:17:PHE:CZ	2:B:83:TYR:HB2	2.55	0.41
2:E:46:GLU:HB2	2:E:62:ASN:OD1	2.20	0.41
2:E:98:LYS:HE2	6:E:215:HOH:O	2.19	0.41
2:E:52:GLU:HG2	6:E:238:HOH:O	2.18	0.41
2:B:158:LEU:HD12	2:B:158:LEU:N	2.35	0.41
2:E:47:TYR:OH	2:E:71:ARG:NH1	2.54	0.41
2:E:97:PRO:HG3	2:E:122:PHE:HB3	2.03	0.41
2:B:152:ASP:O	2:B:153:TRP:HB2	2.20	0.41
2:E:119:VAL:HG11	2:E:127:ILE:CD1	2.51	0.41
1:D:88:GLU:OE2	1:D:111:LYS:HD2	2.21	0.41
1:A:59:ALA:O	1:A:63:ILE:HG12	2.22	0.40
2:B:4:ARG:HA	2:B:5:PRO:HD3	1.95	0.40
2:E:71:ARG:HD3	2:E:71:ARG:HA	1.88	0.40
2:E:81:HIS:CD2	3:F:93:LYS:HG2	2.56	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	179/181 (99%)	176 (98%)	3 (2%)	0	100	100
1	D	179/181 (99%)	177 (99%)	2 (1%)	0	100	100
2	B	189/190 (100%)	174 (92%)	11 (6%)	4 (2%)	5	1
2	E	189/190 (100%)	169 (89%)	17 (9%)	3 (2%)	7	2
3	C	18/20 (90%)	16 (89%)	1 (6%)	1 (6%)	1	0
3	F	16/20 (80%)	15 (94%)	0	1 (6%)	1	0
All	All	770/782 (98%)	727 (94%)	34 (4%)	9 (1%)	10	4

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	135	SER
2	E	134	ASN
2	E	135	SER
2	B	111	HIS
3	C	88	VAL
3	F	88	VAL
2	B	109	LEU
2	E	109	LEU
2	B	165	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	162/166 (98%)	157 (97%)	5 (3%)	35	29
1	D	164/166 (99%)	159 (97%)	5 (3%)	36	30
2	B	159/171 (93%)	155 (98%)	4 (2%)	42	37
2	E	161/171 (94%)	156 (97%)	5 (3%)	35	29
3	C	18/20 (90%)	18 (100%)	0	100	100
3	F	18/20 (90%)	18 (100%)	0	100	100
All	All	682/714 (96%)	663 (97%)	19 (3%)	39	32

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	80	THR
1	A	92	LEU
1	A	123	ARG
1	A	177	HIS
2	B	66	ASP
2	B	98	LYS
2	B	160	MET

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Mol	Chain	Res	Type
2	B	161	LEU
1	D	71	GLU
1	D	92	LEU
1	D	170	LEU
1	D	174	LEU
1	D	177	HIS
2	E	6	ARG
2	E	50	VAL
2	E	66[A]	ASP
2	E	66[B]	ASP
2	E	107	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	ASN
1	A	149	HIS
1	A	167	HIS
2	B	9	GLN
2	B	107	GLN
2	B	113	ASN
2	B	120	ASN
2	B	134	ASN
2	B	174	GLN
1	D	118	ASN
1	D	143	HIS
1	D	149	HIS
1	D	167	HIS
2	E	9	GLN
2	E	92	GLN
2	E	113	ASN
2	E	174	GLN

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 [i](#)

There are no oligosaccharides 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	$\# Z > 2$
4	SO4	B	191	-	4,4,4	0.37	0	6,6,6	0.08	0
4	SO4	D	182	-	4,4,4	0.37	0	6,6,6	0.12	0
5	GOL	B	192	-	5,5,5	1.05	0	5,5,5	1.00	0
5	GOL	D	183	-	5,5,5	1.04	0	5,5,5	1.01	0
4	SO4	A	182	-	4,4,4	0.39	0	6,6,6	0.03	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	192	-	-	4/4/4/4	-
5	GOL	D	183	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	192	GOL	O1-C1-C2-C3
5	B	192	GOL	C1-C2-C3-O3
5	B	192	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	D	183	GOL	C1-C2-C3-O3
5	D	183	GOL	O2-C2-C3-O3
5	B	192	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	182	SO4	1	0
5	B	192	GOL	2	0
5	D	183	GOL	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	179/181 (98%)	-1.32	0 100 100	16, 25, 43, 62	2 (1%)
1	D	178/181 (98%)	-1.37	0 100 100	15, 25, 44, 56	3 (1%)
2	B	190/190 (100%)	-1.11	0 100 100	18, 37, 73, 77	1 (0%)
2	E	190/190 (100%)	-1.17	0 100 100	18, 36, 74, 81	1 (0%)
3	C	20/20 (100%)	-1.02	0 100 100	24, 37, 69, 69	0
3	F	18/20 (90%)	-1.05	0 100 100	23, 33, 60, 68	0
All	All	775/782 (99%)	-1.23	0 100 100	15, 31, 67, 81	7 (0%)

There are no RSRZ outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	A	182	5/5	0.98	0.04	69,69,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	B	191	5/5	0.98	0.04	90,90,90,91	0
4	SO4	D	182	5/5	0.98	0.05	72,72,72,73	0
5	GOL	B	192	6/6	0.98	0.06	47,49,50,52	0
5	GOL	D	183	6/6	0.98	0.05	69,70,70,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.