



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:40 PM UTC

PDB ID : 2R7G / pdb_00002r7g
Title : Structure of the retinoblastoma protein pocket domain in complex with adenovirus E1A CR1 domain
Authors : Liu, X.; Marmorstein, R.
Deposited on : 2007-09-07
Resolution : 1.67 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

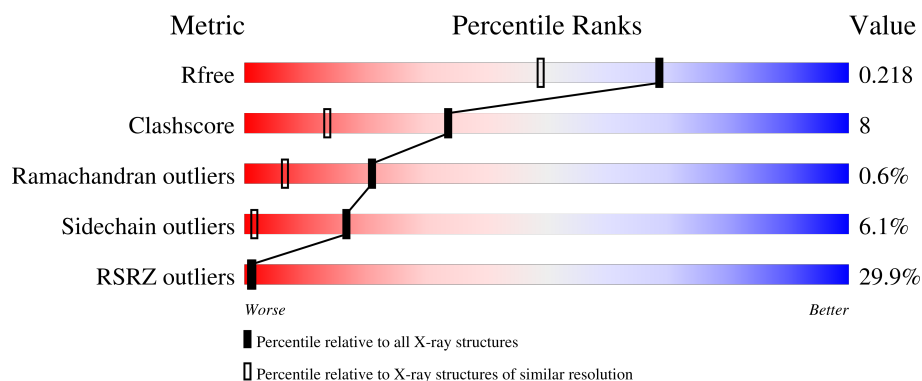
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.67 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}	180053	1054 (1.68-1.68)
Clashscore	190562	1078 (1.68-1.68)
Ramachandran outliers	187476	1068 (1.68-1.68)
Sidechain outliers	187428	1067 (1.68-1.68)
RSRZ outliers	180081	1055 (1.68-1.68)

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	347	33% 77% 17% • •
1	C	347	24% 80% 15% • •
2	B	10	30% 60% 30% 10%
2	D	10	20% 100%
2	E	10	80% 70% 20% 10%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6267 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.

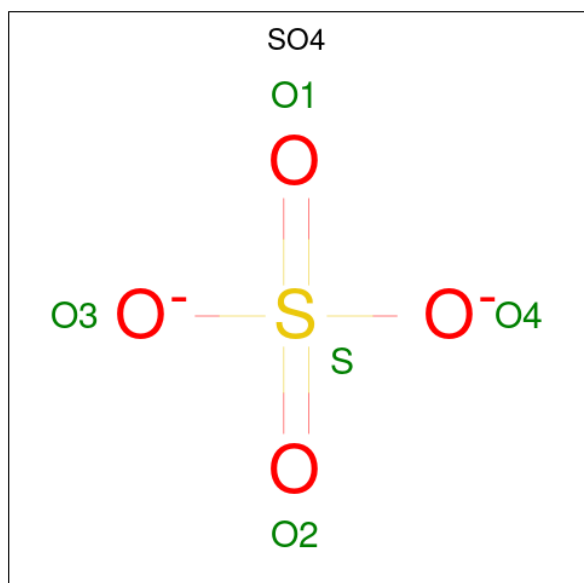
- Molecule 1 is a protein called Retinoblastoma-associated protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2760	1779	463	498	20			
1	C	337	Total	C	N	O	S	0	0	0
			2771	1785	467	499	20			

- Molecule 2 is a protein called Early E1A 32 kDa protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	10	Total	C	N	O	0	0	0
			84	56	12	16			
2	D	10	Total	C	N	O	0	0	0
			84	56	12	16			
2	E	9	Total	C	N	O	0	0	0
			76	50	11	15			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

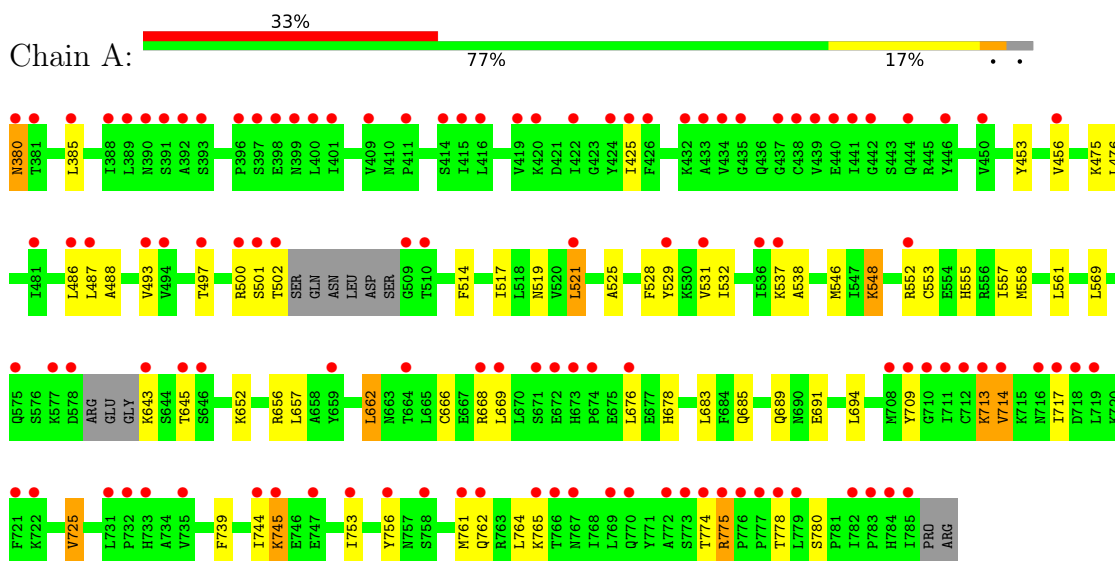
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	232	Total	O	0	0
			232	232		
4	B	7	Total	O	0	0
			7	7		
4	C	234	Total	O	0	0
			234	234		
4	D	7	Total	O	0	0
			7	7		
4	E	2	Total	O	0	0
			2	2		

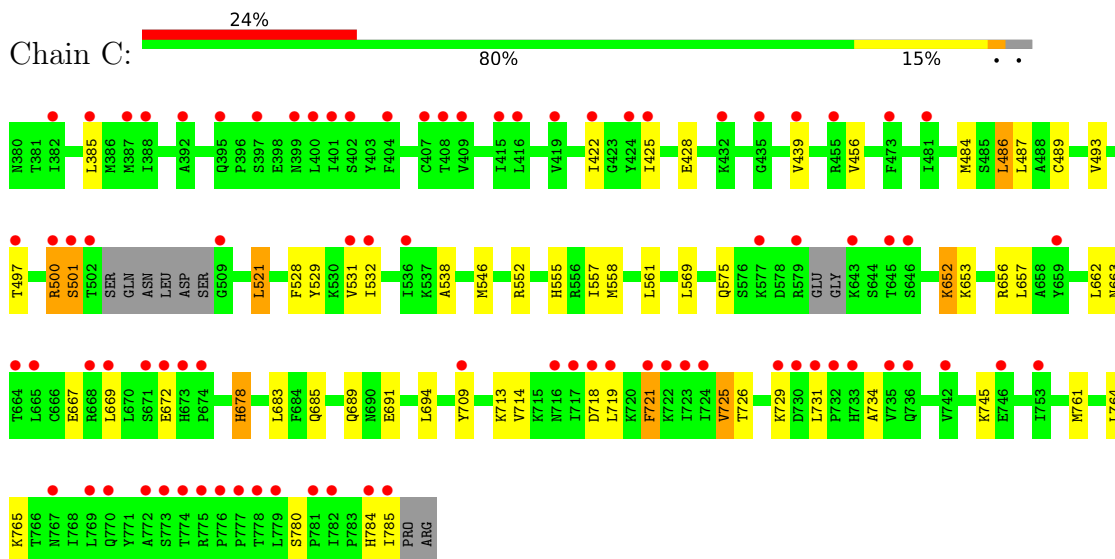
3 Residue-property plots [i](#)

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.

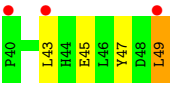
- Molecule 1: Retinoblastoma-associated protein



- Molecule 1: Retinoblastoma-associated protein



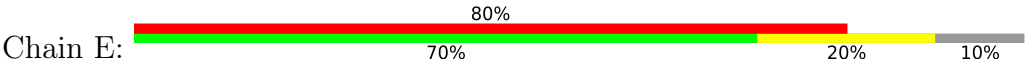
- Molecule 2: Early E1A 32 kDa protein



• Molecule 2: Early E1A 32 kDa protein



• Molecule 2: Early E1A 32 kDa protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.71Å 57.71Å 92.27Å 94.34° 92.69° 105.79°	Depositor
Resolution (Å)	40.82 – 1.67 40.82 – 1.67	Depositor EDS
% Data completeness (in resolution range)	95.2 (40.82-1.67) 87.4 (40.82-1.67)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 1.67Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.195 , 0.218 0.194 , 0.218	Depositor DCC
R_{free} test set	12140 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	21.9	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.012 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6267	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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: 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	0.66	0/2814	0.83	0/3790
1	C	0.66	0/2825	0.81	0/3804
2	B	0.62	0/87	0.81	0/119
2	D	0.66	0/87	0.63	0/119
2	E	0.40	0/79	0.81	0/108
All	All	0.66	0/5892	0.82	0/7940

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2760	0	2814	53	0
1	C	2771	0	2827	38	0
2	B	84	0	80	4	0
2	D	84	0	80	0	0
2	E	76	0	69	3	0
3	A	5	0	0	0	0
3	C	5	0	0	0	0
4	A	232	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	7	0	0	0	0
4	C	234	0	0	4	0
4	D	7	0	0	0	0
4	E	2	0	0	0	0
All	All	6267	0	5870	90	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 8.

All (90) 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:525:ALA:HB1	1:A:557:ILE:HD12	1.42	1.00
1:C:555:HIS:HA	1:C:558:MET:HE2	1.46	0.95
1:A:514:PHE:HZ	1:A:557:ILE:HD11	1.33	0.93
1:C:486:LEU:HD23	1:C:531:VAL:HG11	1.52	0.91
1:C:422:ILE:HD11	1:C:484:MET:SD	2.12	0.88
1:C:528:PHE:CE2	1:C:532:ILE:HD11	2.13	0.84
1:C:663:ASN:O	1:C:667:GLU:HG2	1.78	0.83
1:A:753:ILE:HD12	2:E:48:ASP:HB3	1.61	0.81
1:A:528:PHE:CE2	1:A:532:ILE:HD11	2.17	0.79
1:A:676:LEU:HD11	1:A:717:ILE:HD13	1.63	0.78
1:A:493:VAL:O	1:A:497:THR:HG23	1.85	0.77
1:A:555:HIS:HA	1:A:558:MET:CE	2.16	0.75
1:A:645:THR:HG23	2:B:45:GLU:O	1.87	0.74
1:A:555:HIS:HA	1:A:558:MET:HE2	1.70	0.74
1:A:425:ILE:HG13	1:C:425:ILE:HD11	1.69	0.74
1:A:514:PHE:CZ	1:A:557:ILE:HD11	2.20	0.74
1:C:555:HIS:HA	1:C:558:MET:CE	2.21	0.71
1:C:493:VAL:O	1:C:497:THR:HG23	1.91	0.70
1:C:558:MET:HE3	1:C:657:LEU:HD22	1.73	0.70
1:A:557:ILE:HD13	1:A:561:LEU:HD12	1.73	0.70
1:A:714:VAL:HG13	2:E:43:LEU:HD21	1.73	0.69
1:C:422:ILE:CD1	1:C:484:MET:SD	2.83	0.67
1:C:428:GLU:HG2	4:C:955:HOH:O	1.95	0.66
1:A:537:LYS:HD2	4:A:952:HOH:O	1.96	0.65
1:A:453:TYR:HD1	1:A:486:LEU:HD22	1.62	0.65
1:C:678:HIS:HE1	1:C:780:SER:O	1.80	0.64
1:A:753:ILE:CD1	2:E:48:ASP:HB3	2.27	0.64
1:A:652:LYS:HE2	4:A:915:HOH:O	1.99	0.62
1:A:678:HIS:HE1	1:A:780:SER:O	1.83	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:MET:HE3	1:A:657:LEU:HD22	1.81	0.61
1:C:529:TYR:OH	1:C:653:LYS:HD2	2.03	0.58
1:A:497:THR:HG22	4:A:1117:HOH:O	2.03	0.57
1:A:425:ILE:CG1	1:C:425:ILE:HD11	2.35	0.56
1:C:652:LYS:HE3	1:C:656:ARG:HH22	1.69	0.56
1:A:685:GLN:HE22	1:A:689:GLN:HE21	1.52	0.56
1:A:453:TYR:CD1	1:A:486:LEU:HD22	2.40	0.56
2:B:47:TYR:O	2:B:49:LEU:HD13	2.06	0.54
1:C:685:GLN:HE22	1:C:689:GLN:NE2	2.05	0.54
1:C:709:TYR:CE1	1:C:713:LYS:HE2	2.44	0.53
1:A:380:ASN:HB2	4:A:1021:HOH:O	2.09	0.52
1:A:456:VAL:HG13	1:A:538:ALA:HB3	1.90	0.52
1:A:643:LYS:NZ	4:A:964:HOH:O	2.43	0.52
1:A:685:GLN:HE22	1:A:689:GLN:NE2	2.09	0.51
1:A:486:LEU:HD23	1:A:486:LEU:O	2.10	0.51
1:C:531:VAL:HG12	1:C:531:VAL:O	2.09	0.51
1:A:555:HIS:HA	1:A:558:MET:HE3	1.92	0.50
1:A:497:THR:HG21	1:A:546:MET:HE2	1.93	0.50
1:A:488:ALA:HB2	1:A:521:LEU:HD23	1.93	0.50
1:A:691:GLU:HG3	1:A:764:LEU:HD21	1.92	0.50
1:A:555:HIS:ND1	1:A:558:MET:HE1	2.27	0.49
1:C:497:THR:HG22	4:C:1105:HOH:O	2.13	0.48
1:C:486:LEU:HD23	1:C:531:VAL:CG1	2.33	0.48
1:A:744:ILE:HD12	1:A:744:ILE:N	2.29	0.47
1:C:761:MET:HE3	1:C:765:LYS:HA	1.95	0.47
1:A:553:CYS:O	1:A:557:ILE:HG12	2.14	0.47
1:A:555:HIS:CA	1:A:558:MET:HE2	2.43	0.46
1:C:691:GLU:HG3	1:C:764:LEU:HD21	1.97	0.46
1:A:652:LYS:HE3	1:A:656:ARG:HH12	1.80	0.46
1:A:529:TYR:HB2	1:A:557:ILE:HG21	1.98	0.46
1:C:555:HIS:CA	1:C:558:MET:HE2	2.32	0.45
1:C:652:LYS:CE	1:C:656:ARG:HH22	2.27	0.45
1:A:744:ILE:HG22	1:A:745:LYS:HD3	1.98	0.45
1:C:425:ILE:HD12	1:C:425:ILE:N	2.31	0.45
1:A:548:LYS:HE3	1:A:548:LYS:HB2	1.65	0.44
1:C:484:MET:HE1	1:C:521:LEU:HG	1.99	0.44
1:A:517:ILE:HG13	1:A:521:LEU:HD22	1.99	0.44
1:A:475:LYS:NZ	1:C:575:GLN:HE21	2.14	0.44
1:A:519:ASN:HB3	4:A:959:HOH:O	2.18	0.44
1:C:456:VAL:HG13	1:C:538:ALA:HB3	1.99	0.44
1:C:731:LEU:HB2	1:C:734:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:555:HIS:ND1	1:A:558:MET:CE	2.81	0.43
1:A:756:TYR:CE2	1:A:761:MET:HE2	2.53	0.43
1:C:557:ILE:HA	1:C:561:LEU:HB2	2.00	0.43
1:A:761:MET:HG2	1:A:765:LYS:HB3	1.99	0.43
1:A:531:VAL:HG12	1:A:531:VAL:O	2.19	0.42
1:C:784:HIS:O	1:C:785:ILE:HG13	2.19	0.42
1:C:489:CYS:SG	1:C:532:ILE:HD13	2.59	0.42
1:A:709:TYR:CE1	1:A:713:LYS:HG3	2.54	0.42
1:C:484:MET:CE	1:C:521:LEU:HG	2.49	0.42
1:C:721:PHE:O	1:C:725:VAL:HB	2.19	0.42
1:C:439:VAL:HA	4:C:958:HOH:O	2.20	0.42
1:C:726:THR:O	1:C:729:LYS:HG2	2.20	0.41
1:C:497:THR:HG21	1:C:546:MET:HE2	2.03	0.41
1:A:774:THR:HG23	1:A:775:ARG:HD2	2.02	0.41
1:A:662:LEU:HD22	1:A:666:CYS:SG	2.60	0.41
1:A:725:VAL:HG13	1:A:739:PHE:CZ	2.56	0.41
1:C:500:ARG:HG2	1:C:501:SER:N	2.32	0.41
1:A:475:LYS:HE3	4:C:931:HOH:O	2.19	0.40
1:A:476:LEU:HD21	2:B:43:LEU:HD23	2.03	0.40
2:B:47:TYR:HB2	2:B:49:LEU:HD22	2.02	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	330/347 (95%)	322 (98%)	7 (2%)	1 (0%)	36	21
1	C	331/347 (95%)	324 (98%)	4 (1%)	3 (1%)	14	3
2	B	8/10 (80%)	8 (100%)	0	0	100	100
2	D	8/10 (80%)	8 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	7/10 (70%)	7 (100%)	0	0	100	100
All	All	684/724 (94%)	669 (98%)	11 (2%)	4 (1%)	21	7

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	501	SER
1	C	718	ASP
1	C	501	SER
1	C	719	LEU

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	313/325 (96%)	292 (93%)	21 (7%)	15	1
1	C	314/325 (97%)	296 (94%)	18 (6%)	18	2
2	B	10/10 (100%)	9 (90%)	1 (10%)	7	0
2	D	10/10 (100%)	10 (100%)	0	100	100
2	E	9/10 (90%)	9 (100%)	0	100	100
All	All	656/680 (96%)	616 (94%)	40 (6%)	17	1

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	380	ASN
1	A	385	LEU
1	A	487	LEU
1	A	500	ARG
1	A	502	THR
1	A	521	LEU
1	A	548	LYS
1	A	552	ARG

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Mol	Chain	Res	Type
1	A	569	LEU
1	A	662	LEU
1	A	668	ARG
1	A	669	LEU
1	A	683	LEU
1	A	694	LEU
1	A	713	LYS
1	A	714	VAL
1	A	725	VAL
1	A	745	LYS
1	A	762	GLN
1	A	775	ARG
1	A	778	THR
2	B	49	LEU
1	C	385	LEU
1	C	486	LEU
1	C	487	LEU
1	C	500	ARG
1	C	521	LEU
1	C	552	ARG
1	C	569	LEU
1	C	652	LYS
1	C	662	LEU
1	C	669	LEU
1	C	672	GLU
1	C	678	HIS
1	C	683	LEU
1	C	694	LEU
1	C	714	VAL
1	C	721	PHE
1	C	725	VAL
1	C	745	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	380	ASN
1	A	399	ASN
1	A	406	ASN
1	A	471	GLN
1	A	673	HIS
1	A	678	HIS

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Mol	Chain	Res	Type
1	A	689	GLN
1	A	690	ASN
1	A	716	ASN
1	A	736	GLN
1	C	399	ASN
1	C	406	ASN
1	C	471	GLN
1	C	478	ASN
1	C	575	GLN
1	C	678	HIS
1	C	689	GLN
1	C	690	ASN
1	C	762	GLN
1	C	770	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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](#)

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	$\# Z > 2$
3	SO4	C	901	-	4,4,4	0.56	0	6,6,6	0.42	0
3	SO4	A	902	-	4,4,4	0.22	0	6,6,6	0.46	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	336/347 (96%)	1.57	114 (33%) 1 1	18, 25, 42, 54	0
1	C	337/347 (97%)	1.40	83 (24%) 2 2	19, 25, 44, 53	0
2	B	10/10 (100%)	1.04	3 (30%) 1 1	23, 26, 28, 31	0
2	D	10/10 (100%)	0.77	2 (20%) 3 3	23, 25, 28, 29	0
2	E	9/10 (90%)	3.05	8 (88%) 0 0	37, 39, 41, 42	0
All	All	702/724 (96%)	1.49	210 (29%) 1 1	18, 25, 42, 54	0

All (210) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	48	ASP	7.0
1	A	502	THR	7.0
1	C	502	THR	6.6
1	C	501	SER	6.6
1	A	785	ILE	6.4
1	C	718	ASP	6.0
1	A	774	THR	5.8
1	C	785	ILE	5.8
1	C	716	ASN	5.2
1	A	501	SER	4.9
1	A	777	PRO	4.6
1	C	773	SER	4.5
1	C	382	ILE	4.4
1	A	784	HIS	4.4
1	A	775	ARG	4.4
1	C	778	THR	4.0
1	C	579	ARG	4.0
1	A	441	ILE	4.0
1	A	776	PRO	3.9
1	C	643	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	C	784	HIS	3.8
1	A	732	PRO	3.8
1	C	424	TYR	3.7
1	C	774	THR	3.7
1	A	761	MET	3.7
1	C	723	ILE	3.6
1	C	777	PRO	3.6
1	A	392	ALA	3.6
1	A	772	ALA	3.6
1	A	762	GLN	3.6
1	C	721	PHE	3.6
1	C	717	ILE	3.5
1	C	709	TYR	3.5
1	A	778	THR	3.5
1	A	385	LEU	3.5
1	A	433	ALA	3.4
1	A	401	ILE	3.4
1	A	434	VAL	3.4
1	C	779	LEU	3.3
2	E	40	PRO	3.3
1	A	419	VAL	3.3
2	E	41	PRO	3.3
1	C	399	ASN	3.3
1	A	672	GLU	3.3
2	B	49	LEU	3.2
1	A	735	VAL	3.2
1	C	645	THR	3.2
2	E	46	LEU	3.2
1	A	424	TYR	3.1
1	A	721	PHE	3.1
1	A	440	GLU	3.1
1	C	673	HIS	3.1
1	C	401	ILE	3.1
1	A	731	LEU	3.1
1	C	769	LEU	3.1
1	C	772	ALA	3.1
1	A	388	ILE	3.0
1	C	782	ILE	3.0
1	C	746	GLU	3.0
1	A	733	HIS	3.0
1	C	400	LEU	3.0
1	A	767	ASN	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	494	VAL	3.0
1	A	400	LEU	3.0
1	C	731	LEU	3.0
1	A	674	PRO	3.0
1	C	409	VAL	2.9
1	A	766	THR	2.9
1	A	536	ILE	2.9
2	E	47	TYR	2.9
1	C	425	ILE	2.9
1	C	668	ARG	2.9
1	C	646	SER	2.9
1	A	439	VAL	2.9
1	A	719	LEU	2.9
1	C	536	ILE	2.9
1	C	724	ILE	2.9
1	A	671	SER	2.9
1	A	399	ASN	2.9
1	C	509	GLY	2.8
1	C	753	ILE	2.8
1	A	668	ARG	2.8
1	A	708	MET	2.8
1	A	718	ASP	2.8
1	A	714	VAL	2.8
1	A	398	GLU	2.8
1	A	487	LEU	2.8
1	A	769	LEU	2.8
1	A	645	THR	2.8
1	A	435	GLY	2.8
1	A	745	LYS	2.7
1	A	659	TYR	2.7
1	A	712	CYS	2.7
1	C	719	LEU	2.7
1	A	497	THR	2.7
1	C	736	GLN	2.7
1	A	669	LEU	2.7
1	A	709	TYR	2.7
1	C	767	ASN	2.7
1	C	775	ARG	2.7
1	A	438	CYS	2.7
1	A	396	PRO	2.6
1	A	420	LYS	2.6
1	A	510	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	729	LYS	2.6
2	E	42	THR	2.6
1	A	389	LEU	2.6
1	A	425	ILE	2.6
1	A	717	ILE	2.6
1	A	578	ASP	2.6
1	A	409	VAL	2.6
1	C	659	TYR	2.6
1	C	422	ILE	2.6
1	A	456	VAL	2.6
1	A	509	GLY	2.5
1	C	402	SER	2.5
1	C	415	ILE	2.5
1	A	437	GLY	2.5
1	A	779	LEU	2.5
1	C	416	LEU	2.5
2	E	43	LEU	2.5
1	A	529	TYR	2.5
2	D	40	PRO	2.5
1	A	537	LYS	2.5
1	A	422	ILE	2.5
1	A	747	GLU	2.5
1	A	716	ASN	2.4
1	A	643	LYS	2.4
1	C	455	ARG	2.4
1	A	710	GLY	2.4
1	A	390	ASN	2.4
1	A	391	SER	2.4
1	A	432	LYS	2.4
1	A	426	PHE	2.4
1	C	497	THR	2.4
1	A	446	TYR	2.4
1	C	735	VAL	2.4
1	C	733	HIS	2.4
1	A	773	SER	2.3
1	A	486	LEU	2.3
2	B	43	LEU	2.3
1	A	782	ILE	2.3
1	C	435	GLY	2.3
1	C	385	LEU	2.3
1	A	722	LYS	2.3
1	A	783	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	407	CYS	2.3
1	A	756	TYR	2.3
1	C	481	ILE	2.3
1	C	730	ASP	2.3
1	A	493	VAL	2.3
1	C	674	PRO	2.2
1	C	669	LEU	2.2
2	D	49	LEU	2.2
1	A	397	SER	2.2
1	A	758	SER	2.2
1	A	577	LYS	2.2
1	A	753	ILE	2.2
1	C	388	ILE	2.2
1	C	532	ILE	2.2
1	C	732	PRO	2.2
1	C	776	PRO	2.2
1	A	380	ASN	2.2
1	A	646	SER	2.2
1	A	575	GLN	2.2
1	A	711	ILE	2.2
1	C	408	THR	2.2
1	A	765	LYS	2.2
1	C	531	VAL	2.2
1	C	577	LYS	2.2
1	C	671	SER	2.2
1	C	665	LEU	2.2
1	A	552	ARG	2.2
1	A	411	PRO	2.2
1	C	781	PRO	2.2
2	B	40	PRO	2.2
1	C	439	VAL	2.1
1	C	742	VAL	2.1
1	C	395	GLN	2.1
1	A	416	LEU	2.1
1	A	381	THR	2.1
1	A	500	ARG	2.1
1	A	450	VAL	2.1
1	A	442	GLY	2.1
1	A	713	LYS	2.1
1	C	722	LYS	2.1
1	C	770	GLN	2.1
1	A	664	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	500	ARG	2.1
1	C	664	THR	2.1
1	A	673	HIS	2.1
1	C	432	LYS	2.1
1	A	393	SER	2.1
1	A	414	SER	2.1
1	A	676	LEU	2.1
2	E	44	HIS	2.1
1	C	392	ALA	2.0
1	A	444	GLN	2.0
1	A	531	VAL	2.0
1	C	397	SER	2.0
1	A	521	LEU	2.0
1	C	672	GLU	2.0
1	A	770	GLN	2.0
1	C	387	MET	2.0
1	A	415	ILE	2.0
1	A	481	ILE	2.0
1	A	744	ILE	2.0
1	C	404	PHE	2.0
1	C	473	PHE	2.0
1	C	419	VAL	2.0

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
3	SO4	C	901	5/5	0.97	0.10	20,22,23,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	902	5/5	0.98	0.12	20,21,22,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.