



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:50 PM UTC

PDB ID : 3KHV / pdb_00003khv
Title : Crystal Structures of Urokinase-type Plasminogen Activator in Complex with 4-(Aminomethyl) Benzoic Acid and 4-(Aminomethyl-phenyl)-methanol
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Deposited on : 2009-10-30
Resolution : 2.35 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

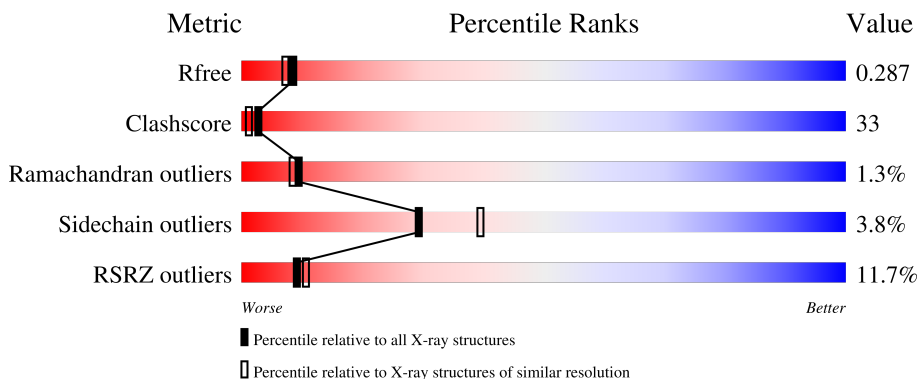
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	253	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	4AL	A	4069	-	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2175 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.

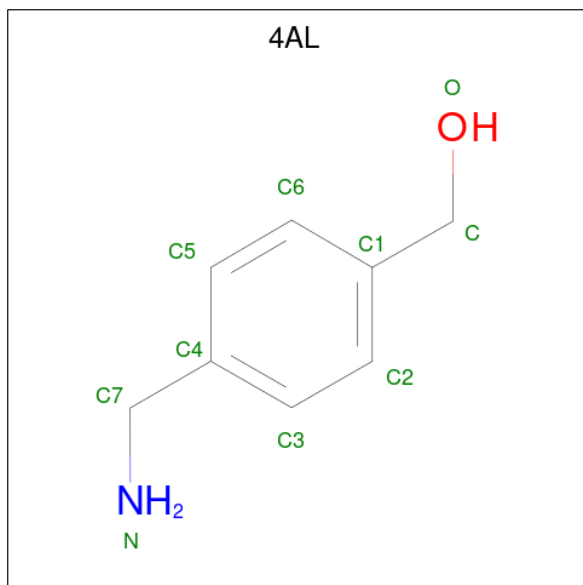
- Molecule 1 is a protein called Urokinase-type plasminogen activator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	239	1890	1196	328	351	15	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	122	ALA	CYS	engineered mutation	UNP P00749
A	145	GLN	ASN	engineered mutation	UNP P00749

- Molecule 2 is [4-(aminomethyl)phenyl]methanol (CCD ID: 4AL) (formula: C₈H₁₁NO).



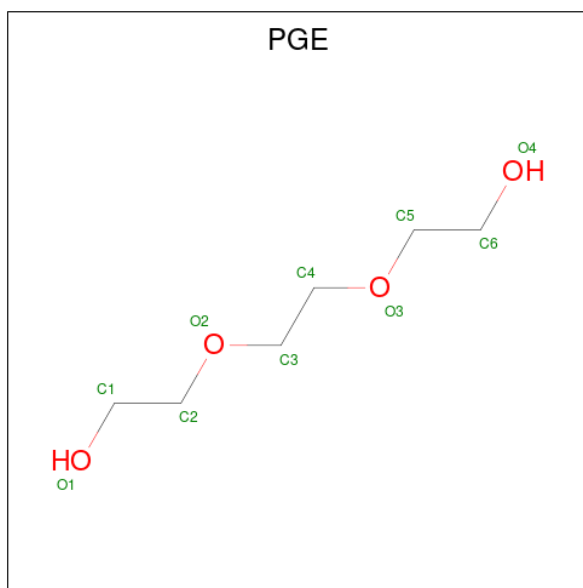
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	10	8	1	1	0	0

- 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		

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	6	4		

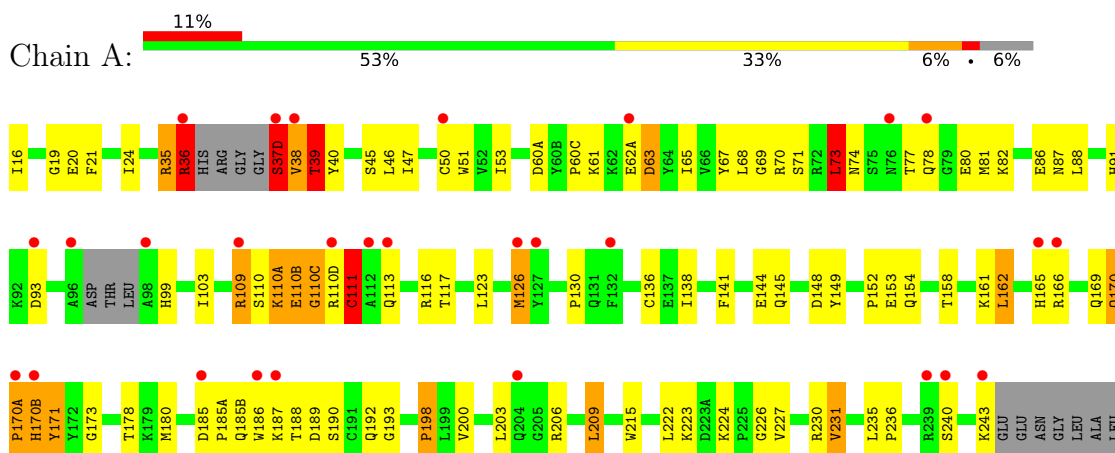
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	260	Total 260	O 260	0	0

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: Urokinase-type plasminogen activator



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	120.83Å 120.83Å 42.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.26 – 2.35 39.26 – 2.35	Depositor EDS
% Data completeness (in resolution range)	96.0 (39.26-2.35) 96.2 (39.26-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 2.34Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.293 0.234 , 0.287	Depositor DCC
R_{free} test set	968 reflections (10.48%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtrriage
Anisotropy	0.387	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 88.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtrriage
Estimated twinning fraction	0.014 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	2175	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.87% 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: PGE, 4AL, 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	1.44	34/1936 (1.8%)	1.22	21/2620 (0.8%)

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

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	CYS	C-O	-20.97	1.02	1.23
1	A	170	GLN	CA-C	-15.52	1.33	1.53
1	A	110	SER	CA-C	-13.35	1.35	1.53
1	A	170	GLN	C-O	-12.66	1.07	1.23
1	A	40	TYR	C-O	-11.68	1.10	1.24
1	A	170(A)	PRO	C-O	-11.21	1.09	1.24
1	A	35	ARG	C-O	-11.12	1.09	1.23
1	A	36	ARG	CZ-NH2	-11.04	1.19	1.33
1	A	36	ARG	C-O	-10.69	1.10	1.23
1	A	39	THR	N-CA	10.50	1.59	1.46
1	A	110(A)	LYS	C-O	-9.35	1.12	1.24
1	A	40	TYR	N-CA	7.91	1.56	1.46
1	A	36	ARG	CA-C	-7.88	1.43	1.53
1	A	170(B)	HIS	N-CA	-7.79	1.36	1.46
1	A	110	SER	C-O	-7.75	1.13	1.23
1	A	170	GLN	CG-CD	-7.54	1.33	1.52
1	A	37(D)	SER	C-N	7.25	1.43	1.33
1	A	110(B)	GLU	C-O	-7.06	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	170(A)	PRO	N-CA	-6.89	1.38	1.47
1	A	39	THR	CB-CG2	-6.88	1.29	1.52
1	A	36	ARG	CZ-NH1	-6.66	1.23	1.32
1	A	111	CYS	CA-C	6.61	1.60	1.53
1	A	170(A)	PRO	CA-C	-6.27	1.43	1.52
1	A	171	TYR	C-O	-6.16	1.16	1.24
1	A	40	TYR	CD1-CE1	-6.16	1.20	1.38
1	A	170	GLN	CB-CG	-6.14	1.34	1.52
1	A	40	TYR	CE2-CZ	-6.10	1.23	1.38
1	A	110(D)	ARG	CG-CD	5.38	1.68	1.52
1	A	40	TYR	C-N	-5.25	1.26	1.33
1	A	36	ARG	NE-CZ	-5.19	1.27	1.33
1	A	35	ARG	C-N	-5.14	1.27	1.33
1	A	170	GLN	N-CA	-5.07	1.37	1.45
1	A	110(C)	GLY	C-O	-5.02	1.16	1.24
1	A	110(B)	GLU	CD-OE2	-5.00	1.15	1.25

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37(D)	SER	CA-C-N	-10.55	102.99	121.97
1	A	37(D)	SER	C-N-CA	-10.55	102.99	121.97
1	A	39	THR	N-CA-C	10.20	132.52	110.80
1	A	110(B)	GLU	N-CA-C	-9.46	102.33	112.93
1	A	111	CYS	CA-CB-SG	8.10	133.03	114.40
1	A	36	ARG	N-CA-C	7.59	121.76	108.56
1	A	231	VAL	N-CA-C	7.58	118.35	110.62
1	A	40	TYR	N-CA-CB	6.39	119.55	109.71
1	A	171	TYR	N-CA-C	6.21	124.02	110.80
1	A	111	CYS	O-C-N	-6.10	113.79	121.78
1	A	198	PRO	N-CA-C	6.08	120.45	110.55
1	A	144	GLU	N-CA-C	-5.98	105.98	113.28
1	A	185(A)	PRO	N-CA-C	-5.93	105.93	114.18
1	A	110(C)	GLY	N-CA-C	5.90	124.79	114.76
1	A	36	ARG	NE-CZ-NH1	5.77	127.27	121.50
1	A	73	LEU	N-CA-C	5.61	117.20	111.14
1	A	39	THR	CB-CA-C	-5.56	99.36	110.42
1	A	36	ARG	NE-CZ-NH2	-5.47	114.28	119.20
1	A	149	TYR	N-CA-C	-5.33	106.83	113.55
1	A	37(D)	SER	O-C-N	-5.10	115.81	122.59
1	A	226	GLY	N-CA-C	-5.07	101.43	111.31

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	37(D)	SER	Mainchain

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	1890	0	1847	124	3
2	A	10	0	10	2	0
3	A	5	0	0	0	0
4	A	10	0	14	1	0
5	A	260	0	0	42	13
All	All	2175	0	1871	124	13

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 33.

All (124) 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:38:VAL:O	1:A:39:THR:CG2	1.76	1.33
1:A:37(D):SER:O	1:A:38:VAL:CB	1.81	1.23
1:A:240:SER:HA	1:A:243:LYS:HE3	1.34	1.08
1:A:38:VAL:C	1:A:39:THR:HG23	1.79	1.04
1:A:50:CYS:CB	1:A:111:CYS:SG	2.45	1.04
1:A:36:ARG:C	1:A:37(D):SER:N	2.19	0.99
1:A:187:LYS:HG2	5:A:297:HOH:O	1.62	0.97
1:A:38:VAL:O	1:A:39:THR:HG23	0.80	0.97
1:A:81:MET:HE1	1:A:113:GLN:H	1.29	0.93
1:A:37(D):SER:O	1:A:38:VAL:HB	1.09	0.91
1:A:185:ASP:HB2	5:A:434:HOH:O	1.72	0.89
1:A:185:ASP:HB3	5:A:297:HOH:O	1.73	0.86
1:A:193:GLY:HA2	5:A:464:HOH:O	1.77	0.85
1:A:185:ASP:O	5:A:299:HOH:O	1.93	0.84
1:A:61:LYS:HE2	1:A:62(A):GLU:HB2	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:HIS:HD2	1:A:93:ASP:H	1.25	0.80
1:A:24:ILE:HG12	1:A:69:GLY:HA2	1.65	0.78
1:A:203:LEU:HA	5:A:481:HOH:O	1.86	0.76
1:A:86:GLU:O	1:A:87:ASN:ND2	2.17	0.76
1:A:70:ARG:CZ	5:A:490:HOH:O	2.34	0.76
1:A:145:GLN:HA	5:A:438:HOH:O	1.86	0.75
1:A:170:GLN:HB3	1:A:170(A):PRO:CD	2.17	0.74
1:A:16:ILE:HD13	1:A:190:SER:HA	1.69	0.74
1:A:145:GLN:HB3	5:A:432:HOH:O	1.88	0.73
1:A:45:SER:OG	1:A:198:PRO:HB3	1.88	0.73
1:A:81:MET:HE1	1:A:113:GLN:N	2.04	0.72
1:A:130:PRO:HG3	1:A:203:LEU:HG	1.72	0.71
1:A:37(D):SER:O	1:A:38:VAL:CG2	2.39	0.71
1:A:209:LEU:HD13	1:A:231:VAL:HG21	1.73	0.70
1:A:161:LYS:HD2	5:A:483:HOH:O	1.91	0.69
1:A:145:GLN:OE1	5:A:469:HOH:O	2.12	0.68
1:A:36:ARG:HH11	1:A:65:ILE:HG12	1.58	0.68
1:A:240:SER:HA	1:A:243:LYS:CE	2.19	0.66
1:A:170:GLN:OE1	1:A:170(B):HIS:CE1	2.49	0.66
1:A:38:VAL:HG23	5:A:435:HOH:O	1.94	0.65
1:A:116:ARG:NH1	5:A:390:HOH:O	2.29	0.65
1:A:185:ASP:CB	5:A:297:HOH:O	2.40	0.65
1:A:236:PRO:HD3	5:A:386:HOH:O	1.99	0.62
1:A:185(B):GLN:HB2	5:A:297:HOH:O	2.00	0.61
1:A:73:LEU:HD12	1:A:74:ASN:ND2	2.15	0.61
1:A:24:ILE:N	1:A:71:SER:OG	2.34	0.61
1:A:186:TRP:N	5:A:299:HOH:O	2.31	0.61
1:A:240:SER:CA	1:A:243:LYS:HE3	2.22	0.60
1:A:190:SER:OG	2:A:4069:4AL:HA	2.00	0.60
1:A:21:PHE:N	5:A:259:HOH:O	2.04	0.60
1:A:206:ARG:HA	5:A:316:HOH:O	2.02	0.60
1:A:169:GLN:O	1:A:173:GLY:HA2	2.02	0.59
1:A:77:THR:O	1:A:80:GLU:HG2	2.03	0.59
1:A:82:LYS:N	5:A:8:HOH:O	2.24	0.58
1:A:110(A):LYS:C	1:A:110(C):GLY:H	2.09	0.58
1:A:166:ARG:HA	5:A:330:HOH:O	2.03	0.58
1:A:243:LYS:C	5:A:273:HOH:O	2.46	0.58
1:A:99:HIS:O	1:A:180:MET:HE2	2.04	0.58
1:A:116:ARG:CZ	5:A:390:HOH:O	2.53	0.57
1:A:170:GLN:OE1	1:A:170(B):HIS:HE1	1.87	0.57
1:A:91:HIS:CD2	1:A:93:ASP:H	2.15	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LYS:HE2	1:A:62(A):GLU:CB	2.32	0.56
1:A:165:HIS:O	1:A:169:GLN:HB2	2.06	0.56
1:A:24:ILE:CG2	1:A:117:THR:HB	2.36	0.55
1:A:70:ARG:NH1	5:A:490:HOH:O	2.40	0.55
1:A:166:ARG:NE	5:A:443:HOH:O	2.40	0.55
1:A:236:PRO:CD	5:A:386:HOH:O	2.53	0.55
1:A:185:ASP:O	4:A:5115:PGE:H3	2.06	0.55
1:A:185:ASP:CG	5:A:297:HOH:O	2.50	0.55
1:A:170(B):HIS:CE1	5:A:383:HOH:O	2.60	0.54
1:A:188:THR:O	1:A:189:ASP:HB2	2.08	0.53
1:A:170:GLN:CB	1:A:170(A):PRO:CD	2.79	0.53
1:A:69:GLY:HA2	1:A:117:THR:O	2.09	0.53
1:A:77:THR:HG23	5:A:274:HOH:O	2.08	0.53
1:A:145:GLN:HB2	1:A:148:ASP:CG	2.34	0.52
1:A:53:ILE:HD11	1:A:103:ILE:HD11	1.91	0.52
1:A:206:ARG:NH2	5:A:444:HOH:O	2.43	0.52
1:A:35:ARG:HG3	1:A:63:ASP:O	2.10	0.51
1:A:126:MET:HG2	1:A:235:LEU:HD12	1.92	0.51
1:A:67:TYR:O	1:A:68:LEU:HD23	2.11	0.51
1:A:192:GLN:HA	2:A:4069:4AL:H7	1.91	0.51
1:A:21:PHE:CD2	1:A:154:GLN:HB3	2.46	0.50
1:A:170:GLN:CB	1:A:170(A):PRO:HD3	2.41	0.50
1:A:46:LEU:HD22	1:A:68:LEU:HD13	1.93	0.50
1:A:222:LEU:HD21	5:A:290:HOH:O	2.11	0.49
1:A:136:CYS:HB3	1:A:200:VAL:O	2.13	0.49
1:A:215:TRP:CZ2	1:A:227:VAL:HG21	2.49	0.48
1:A:36:ARG:HD2	1:A:65:ILE:HD11	1.95	0.48
1:A:20:GLU:HB2	5:A:259:HOH:O	2.13	0.48
1:A:24:ILE:HG21	1:A:117:THR:HB	1.95	0.48
1:A:145:GLN:CB	5:A:432:HOH:O	2.54	0.48
1:A:186:TRP:CA	5:A:299:HOH:O	2.62	0.47
1:A:109:ARG:O	1:A:109:ARG:HG3	2.13	0.47
1:A:21:PHE:O	5:A:439:HOH:O	2.20	0.47
1:A:73:LEU:HD12	1:A:74:ASN:HD21	1.79	0.46
1:A:235:LEU:N	5:A:386:HOH:O	2.46	0.46
1:A:222:LEU:HG	5:A:283:HOH:O	2.16	0.46
1:A:24:ILE:HG12	1:A:69:GLY:CA	2.39	0.45
1:A:24:ILE:HG23	1:A:117:THR:HB	1.98	0.45
1:A:47:ILE:HG21	1:A:123:LEU:HD21	1.97	0.45
1:A:145:GLN:HB2	1:A:148:ASP:OD2	2.16	0.45
1:A:185(B):GLN:HB2	1:A:187:LYS:HG2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:SER:O	1:A:243:LYS:HG3	2.17	0.45
1:A:38:VAL:O	1:A:39:THR:CB	2.51	0.44
1:A:24:ILE:H	1:A:71:SER:HG	1.63	0.44
1:A:223:LYS:O	1:A:224:LYS:HG2	2.17	0.44
1:A:186:TRP:HA	5:A:299:HOH:O	2.17	0.44
1:A:130:PRO:HB2	1:A:162:LEU:CD2	2.48	0.43
1:A:188:THR:CG2	5:A:434:HOH:O	2.65	0.43
1:A:46:LEU:HD12	1:A:51:TRP:O	2.18	0.43
1:A:60(C):PRO:O	1:A:88:LEU:HD23	2.18	0.43
1:A:35:ARG:CG	1:A:36:ARG:N	2.81	0.43
1:A:126:MET:HE3	1:A:126:MET:HB3	1.62	0.43
1:A:141:PHE:O	1:A:152:PRO:HD2	2.19	0.43
1:A:178:THR:O	1:A:230:ARG:HD3	2.18	0.42
1:A:138:ILE:HD11	1:A:158:THR:CG2	2.48	0.42
1:A:74:ASN:N	1:A:153:GLU:OE2	2.45	0.42
1:A:110(A):LYS:C	1:A:110(C):GLY:N	2.74	0.42
1:A:36:ARG:HD2	1:A:65:ILE:CG1	2.50	0.41
1:A:86:GLU:C	1:A:87:ASN:ND2	2.77	0.41
1:A:206:ARG:NE	5:A:358:HOH:O	2.53	0.41
1:A:60(A):ASP:C	1:A:60(C):PRO:HD3	2.46	0.41
1:A:215:TRP:CH2	1:A:227:VAL:HG21	2.56	0.41
1:A:73:LEU:HD13	1:A:73:LEU:C	2.46	0.41
1:A:185:ASP:C	5:A:299:HOH:O	2.55	0.41
1:A:186:TRP:N	5:A:297:HOH:O	2.54	0.41
1:A:38:VAL:C	1:A:39:THR:CG2	2.58	0.40
1:A:35:ARG:HA	1:A:63:ASP:O	2.21	0.40
1:A:19:GLY:HA3	1:A:158:THR:HB	2.03	0.40

All (13) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:300:HOH:O	5:A:313:HOH:O[1_556]	1.24	0.96
5:A:257:HOH:O	5:A:399:HOH:O[6_465]	1.37	0.83
5:A:9:HOH:O	5:A:399:HOH:O[6_465]	1.44	0.76
5:A:382:HOH:O	5:A:382:HOH:O[2_665]	1.59	0.61
5:A:259:HOH:O	5:A:469:HOH:O[6_465]	1.84	0.36
1:A:110(B):GLU:OE2	5:A:415:HOH:O[8_665]	1.91	0.29
1:A:78:GLN:NE2	5:A:438:HOH:O[8_665]	2.04	0.16
5:A:15:HOH:O	5:A:390:HOH:O[6_464]	2.09	0.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:GLN:O	5:A:482:HOH:O[8_665]	2.10	0.10
5:A:458:HOH:O	5:A:482:HOH:O[8_665]	2.10	0.10
5:A:355:HOH:O	5:A:375:HOH:O[8_664]	2.13	0.07
5:A:3:HOH:O	5:A:310:HOH:O[1_556]	2.19	0.01
5:A:439:HOH:O	5:A:465:HOH:O[8_664]	2.19	0.01

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	233/253 (92%)	213 (91%)	17 (7%)	3 (1%)	9 8

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	THR
1	A	171	TYR
1	A	38	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	209/219 (95%)	201 (96%)	8 (4%)	29 39

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	63	ASP
1	A	73	LEU
1	A	109	ARG
1	A	111	CYS
1	A	126	MET
1	A	162	LEU
1	A	209	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	ASN
1	A	87	ASN
1	A	91	HIS
1	A	113	GLN
1	A	119	GLN
1	A	131	GLN
1	A	170(B)	HIS
1	A	204	GLN
1	A	233	HIS
1	A	241	HIS

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](#)

3 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	A	402	-	4,4,4	0.33	0	6,6,6	0.13	0
4	PGE	A	5115	-	9,9,9	0.81	0	8,8,8	4.64	1 (12%)
2	4AL	A	4069	-	10,10,10	3.39	6 (60%)	12,12,12	3.08	5 (41%)

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
4	PGE	A	5115	-	-	2/7/7/7	-
2	4AL	A	4069	-	-	0/4/4/4	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	4069	4AL	C3-C2	-5.61	1.29	1.38
2	A	4069	4AL	C3-C4	-4.97	1.29	1.38
2	A	4069	4AL	C-C1	-3.89	1.38	1.51
2	A	4069	4AL	O-C	-3.82	1.25	1.41
2	A	4069	4AL	C2-C1	-3.31	1.32	1.38
2	A	4069	4AL	C6-C1	-3.17	1.32	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	5115	PGE	O2-C2-C1	13.02	167.48	110.11
2	A	4069	4AL	C3-C2-C1	6.06	128.97	121.00
2	A	4069	4AL	O-C-C1	-4.90	94.84	112.07
2	A	4069	4AL	C5-C6-C1	-4.64	114.90	121.00
2	A	4069	4AL	C2-C3-C4	-3.89	115.88	121.00
2	A	4069	4AL	C6-C5-C4	3.15	125.14	121.00

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	5115	PGE	O1-C1-C2-O2
4	A	5115	PGE	O2-C3-C4-O3

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5115	PGE	1	0
2	A	4069	4AL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	239/253 (94%)	0.82	28 (11%) 9 11	13, 29, 68, 104	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	38	VAL	7.8
1	A	37(D)	SER	5.6
1	A	96	ALA	3.4
1	A	98	ALA	3.3
1	A	187	LYS	3.3
1	A	132	PHE	3.2
1	A	78	GLN	3.2
1	A	165	HIS	3.2
1	A	204	GLN	3.1
1	A	113	GLN	2.9
1	A	185	ASP	2.9
1	A	243	LYS	2.9
1	A	109	ARG	2.8
1	A	240	SER	2.8
1	A	62(A)	GLU	2.8
1	A	126	MET	2.8
1	A	110(D)	ARG	2.8
1	A	166	ARG	2.6
1	A	170(B)	HIS	2.5
1	A	170(A)	PRO	2.5
1	A	186	TRP	2.4
1	A	239	ARG	2.4
1	A	93	ASP	2.3
1	A	36	ARG	2.3
1	A	112	ALA	2.2
1	A	127	TYR	2.1
1	A	76	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	50	CYS	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(\AA^2)	Q<0.9
4	PGE	A	5115	10/10	0.82	0.14	29,40,48,49	0
2	4AL	A	4069	10/10	0.88	0.13	39,49,51,56	0
3	SO4	A	402	5/5	0.93	0.11	39,46,50,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.