



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:01 AM UTC

PDB ID : 4OV6 / pdb_00004ov6
Title : Crystal structure of PCSK9(53-451) with Adnectin
Authors : Khan, J.A.
Deposited on : 2014-02-20
Resolution : 2.69 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:

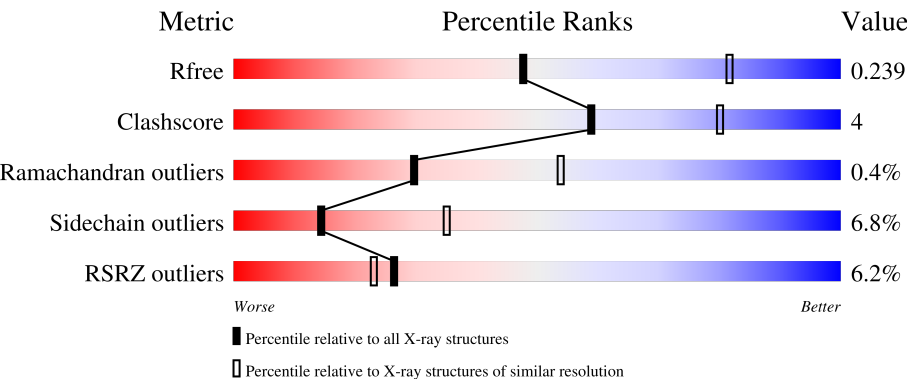
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	93	5% 91% 8%
1	D	93	2% 90% 9%
2	B	294	5% 81% 13%
2	E	294	3% 76% 14% 8%
3	F	99	3% 83% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	G	99	23% 73% 19% 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7181 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 Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	92	Total	C	N	O	S	0	0	0
			730	468	131	129	2			
1	D	93	Total	C	N	O	S	0	0	0
			739	474	133	130	2			

- Molecule 2 is a protein called Proprotein convertase subtilisin/kexin type 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	281	Total	C	N	O	S	0	0	0
			2069	1293	367	398	11			
2	E	270	Total	C	N	O	S	0	0	0
			1988	1242	351	384	11			

- Molecule 3 is a protein called Adnectin.

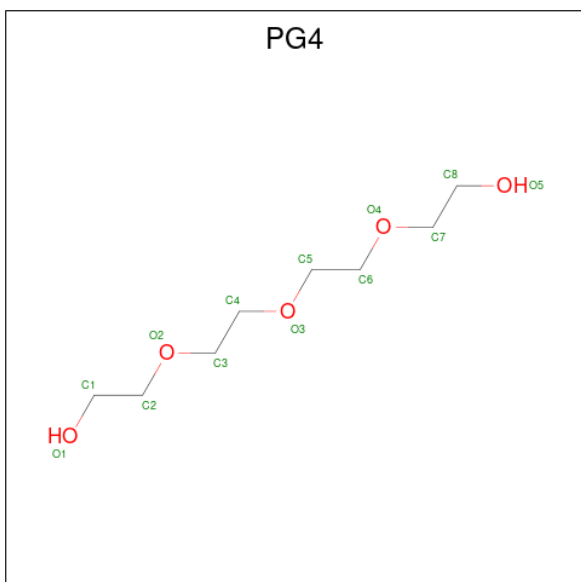
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	99	Total	C	N	O	0	0	0
			759	493	120	146			
3	G	96	Total	C	N	O	0	0	0
			720	467	118	135			

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			13	8	5		
5	D	1	Total	C	O	0	0
			13	8	5		

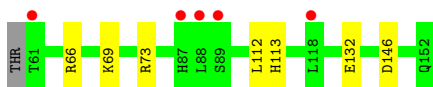
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	10	Total	O	0	0
			10	10		
6	B	38	Total	O	0	0
			38	38		
6	D	10	Total	O	0	0
			10	10		
6	E	36	Total	O	0	0
			36	36		
6	F	23	Total	O	0	0
			23	23		
6	G	13	Total	O	0	0
			13	13		

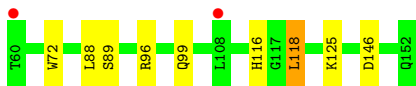
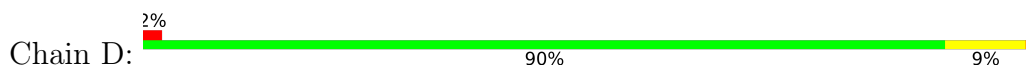
3 Residue-property plots [i](#)

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.

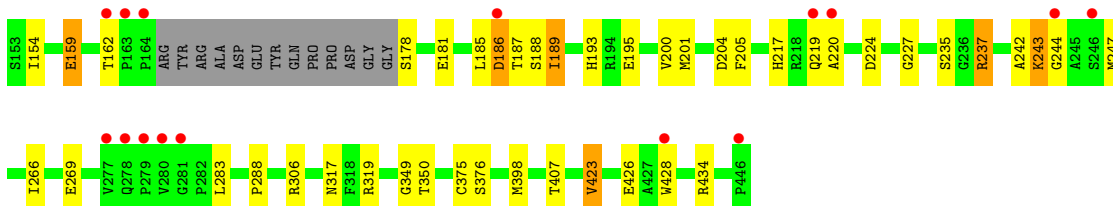
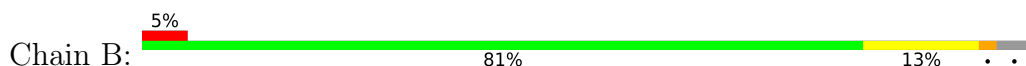
- Molecule 1: Proprotein convertase subtilisin/kexin type 9



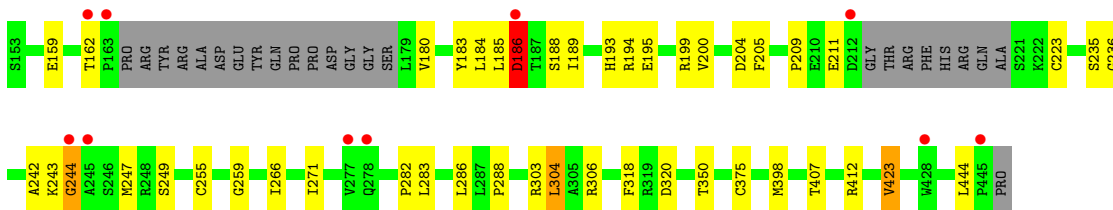
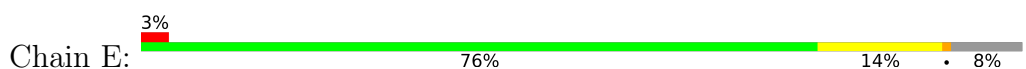
- Molecule 1: Proprotein convertase subtilisin/kexin type 9



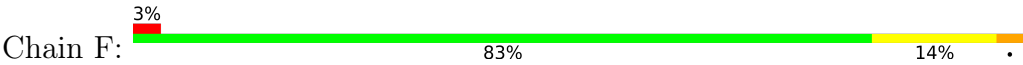
- Molecule 2: Proprotein convertase subtilisin/kexin type 9



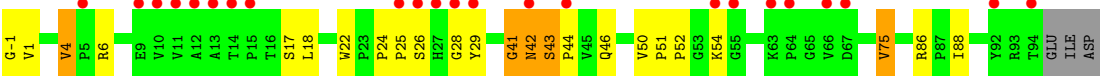
- Molecule 2: Proprotein convertase subtilisin/kexin type 9



- Molecule 3: Adnectin



● Molecule 3: Adnectin



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	75.20Å 118.60Å 168.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.04 – 2.69 22.04 – 2.69	Depositor EDS
% Data completeness (in resolution range)	98.3 (22.04-2.69) 98.0 (22.04-2.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.68Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.11.4, BUSTER 2.11.4	Depositor
R, R_{free}	0.199 , 0.231 0.205 , 0.239	Depositor DCC
R_{free} test set	2116 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	44.7	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7181	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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: EDO, PG4

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	0.80	0/747	1.29	3/1011 (0.3%)
1	D	0.85	0/756	1.27	1/1023 (0.1%)
2	B	0.89	0/2105	1.36	8/2867 (0.3%)
2	E	0.86	0/2019	1.33	9/2748 (0.3%)
3	F	0.85	1/786 (0.1%)	1.23	5/1082 (0.5%)
3	G	0.87	4/746 (0.5%)	1.20	5/1029 (0.5%)
All	All	0.86	5/7159 (0.1%)	1.30	31/9760 (0.3%)

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
2	B	0	1
2	E	0	1
3	G	0	3
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	86	ARG	C-N	6.14	1.41	1.33
3	G	43	SER	C-N	5.84	1.41	1.33
3	G	4	VAL	CA-C	5.53	1.58	1.52
3	F	4	VAL	CA-C	5.07	1.58	1.52
3	G	44	PRO	N-CD	5.01	1.54	1.47

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	162	THR	CB-CA-C	7.10	117.94	109.85
3	G	86	ARG	CA-C-N	-6.72	113.38	120.03
3	G	86	ARG	C-N-CA	-6.72	113.38	120.03
2	E	350	THR	N-CA-C	-6.59	104.87	113.17
2	E	162	THR	CB-CA-C	6.56	117.33	109.85
2	B	350	THR	N-CA-C	-6.53	104.95	113.17
2	B	219	GLN	CA-C-N	6.46	129.77	120.79
2	B	219	GLN	C-N-CA	6.46	129.77	120.79
3	G	43	SER	CA-C-N	-6.36	113.22	119.76
3	G	43	SER	C-N-CA	-6.36	113.22	119.76
2	B	423	VAL	N-CA-CB	-6.30	103.61	112.12
2	E	423	VAL	N-CA-CB	-5.99	104.04	112.12
2	E	236	GLY	CA-C-N	5.88	128.47	120.54
2	E	236	GLY	C-N-CA	5.88	128.47	120.54
1	A	146	ASP	CA-CB-CG	5.84	118.44	112.60
2	B	423	VAL	CB-CA-C	5.73	116.27	110.65
2	E	159	GLU	CA-C-N	5.45	127.89	120.54
2	E	159	GLU	C-N-CA	5.45	127.89	120.54
2	E	423	VAL	CB-CA-C	5.44	115.98	110.65
2	B	159	GLU	N-CA-C	-5.43	104.77	111.40
3	F	29	TYR	CA-C-N	5.40	131.42	121.70
3	F	29	TYR	C-N-CA	5.40	131.42	121.70
1	D	146	ASP	CA-CB-CG	5.31	117.91	112.60
3	F	75	VAL	N-CA-CB	-5.26	102.08	111.92
1	A	132	GLU	CA-C-N	5.17	127.47	120.65
1	A	132	GLU	C-N-CA	5.17	127.47	120.65
3	F	40	GLY	CA-C-N	5.16	131.51	121.41
3	F	40	GLY	C-N-CA	5.16	131.51	121.41
3	G	75	VAL	N-CA-CB	-5.13	102.33	111.92
2	B	317	ASN	CA-CB-CG	5.02	117.62	112.60
2	E	320	ASP	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	244	GLY	Peptide
2	E	244	GLY	Peptide
3	G	26	SER	Peptide
3	G	41	GLY	Peptide
3	G	42	ASN	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	730	0	725	5	0
1	D	739	0	741	6	0
2	B	2069	0	2053	24	0
2	E	1988	0	1978	20	0
3	F	759	0	725	4	0
3	G	720	0	676	10	0
4	A	4	0	6	0	0
4	B	8	0	12	0	0
4	E	8	0	12	0	0
5	B	13	0	18	0	0
5	D	13	0	18	1	0
6	A	10	0	0	0	0
6	B	38	0	0	0	0
6	D	10	0	0	0	0
6	E	36	0	0	0	0
6	F	23	0	0	1	0
6	G	13	0	0	0	0
All	All	7181	0	6964	59	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 4.

All (59) 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:E:199:ARG:HD2	2:E:244:GLY:O	1.76	0.86
2:E:186:ASP:OD1	2:E:288:PRO:HG2	1.92	0.70
2:B:193:HIS:HD2	2:B:195:GLU:H	1.40	0.68
2:B:186:ASP:OD2	2:B:227:GLY:HA2	1.92	0.68
2:E:193:HIS:HD2	2:E:195:GLU:H	1.42	0.67
2:B:200:VAL:HG22	2:B:247:MET:HB2	1.78	0.65
2:B:217:HIS:CE1	1:D:99:GLN:HE22	2.15	0.64
2:E:184:LEU:HD23	2:E:189:ILE:HD11	1.80	0.63
1:A:112:LEU:CD2	2:E:204:ASP:HB3	2.29	0.63
2:B:188:SER:O	2:B:224:ASP:HA	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:185:LEU:O	2:B:288:PRO:HD2	2.04	0.58
1:A:112:LEU:HD23	2:E:204:ASP:HB3	1.85	0.57
3:G:41:GLY:HA2	3:G:42:ASN:CB	2.35	0.57
2:B:189:ILE:CD1	2:B:200:VAL:HG11	2.37	0.54
2:B:186:ASP:CG	2:B:187:THR:H	2.16	0.54
2:B:319:ARG:HG3	2:B:428:TRP:CH2	2.42	0.54
1:A:113:HIS:HE1	2:B:269:GLU:OE1	1.92	0.53
2:E:189:ILE:HD12	2:E:249:SER:HB2	1.91	0.53
1:D:125:LYS:HG2	5:D:201:PG4:H22	1.92	0.52
2:B:189:ILE:HD13	2:B:200:VAL:HG11	1.91	0.52
2:B:235:SER:HA	2:B:242:ALA:O	2.09	0.52
2:E:200:VAL:HG22	2:E:247:MET:HB2	1.93	0.51
3:G:-1:GLY:HA2	3:G:29:TYR:CZ	2.46	0.51
2:B:186:ASP:OD2	2:B:227:GLY:CA	2.60	0.50
2:E:180:VAL:HG22	2:E:282:PRO:HG2	1.95	0.48
2:B:204:ASP:OD1	1:D:116:HIS:HB2	2.14	0.48
1:A:113:HIS:CE1	2:B:269:GLU:OE1	2.66	0.47
3:F:51:PRO:HG2	3:F:54:LYS:HE3	1.97	0.47
1:A:66:ARG:HD3	1:A:73:ARG:CZ	2.45	0.47
2:B:217:HIS:HE1	1:D:99:GLN:HE22	1.58	0.47
2:B:242:ALA:HB2	2:B:398:MET:HG2	1.96	0.47
2:B:220:ALA:HB1	3:F:29:TYR:CE1	2.50	0.47
2:B:237:ARG:O	2:B:243:LYS:HG2	2.16	0.46
2:E:242:ALA:HB2	2:E:398:MET:HG2	1.96	0.46
3:F:1:VAL:HA	3:F:29:TYR:O	2.14	0.46
2:E:184:LEU:HD13	2:E:286:LEU:HD23	1.98	0.46
3:G:41:GLY:HA3	3:G:43:SER:H	1.80	0.46
3:G:25:PRO:CG	3:G:52:PRO:HB2	2.46	0.45
3:G:-1:GLY:HA2	3:G:29:TYR:CE1	2.51	0.45
3:G:41:GLY:CA	3:G:43:SER:H	2.31	0.44
2:B:205:PHE:HE1	2:B:266:ILE:HG22	1.82	0.44
1:D:118:LEU:HD23	1:D:118:LEU:HA	1.85	0.44
2:E:185:LEU:O	2:E:288:PRO:HD2	2.18	0.43
2:E:183:TYR:CD2	2:E:271:ILE:HG12	2.53	0.43
2:B:154:ILE:HD11	2:B:159:GLU:HA	2.00	0.43
2:E:205:PHE:HE1	2:E:266:ILE:HG22	1.83	0.43
3:G:22:TRP:O	3:G:24:PRO:HD3	2.19	0.43
3:G:51:PRO:HD2	3:G:54:LYS:HG3	2.01	0.43
2:E:223:CYS:HG	2:E:255:CYS:HG	0.44	0.43
2:B:349:GLY:HA3	6:F:111:HOH:O	2.18	0.43
2:E:209:PRO:HD3	2:E:259:GLY:HA2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1:VAL:HA	3:G:29:TYR:O	2.19	0.42
2:E:235:SER:HA	2:E:242:ALA:O	2.19	0.42
2:B:220:ALA:HB1	3:F:29:TYR:CD1	2.56	0.41
2:B:426:GLU:HB2	2:B:434:ARG:HG2	2.03	0.41
1:D:72:TRP:HH2	2:E:318:PHE:CE1	2.38	0.41
3:G:41:GLY:CA	3:G:42:ASN:CB	2.99	0.40
2:E:304:LEU:HD12	2:E:304:LEU:HA	1.92	0.40
2:E:189:ILE:HG21	2:E:200:VAL:HG11	2.03	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	90/93 (97%)	87 (97%)	3 (3%)	0	100	100
1	D	91/93 (98%)	86 (94%)	5 (6%)	0	100	100
2	B	277/294 (94%)	268 (97%)	8 (3%)	1 (0%)	30	54
2	E	264/294 (90%)	253 (96%)	10 (4%)	1 (0%)	30	54
3	F	97/99 (98%)	90 (93%)	6 (6%)	1 (1%)	12	32
3	G	94/99 (95%)	90 (96%)	3 (3%)	1 (1%)	11	29
All	All	913/972 (94%)	874 (96%)	35 (4%)	4 (0%)	30	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	F	41	GLY
3	G	28	GLY
2	B	186	ASP
2	E	186	ASP

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	75/80 (94%)	74 (99%)	1 (1%)	61	83
1	D	77/80 (96%)	73 (95%)	4 (5%)	21	47
2	B	221/236 (94%)	209 (95%)	12 (5%)	20	45
2	E	213/236 (90%)	199 (93%)	14 (7%)	15	36
3	F	81/84 (96%)	70 (86%)	11 (14%)	3	9
3	G	73/84 (87%)	65 (89%)	8 (11%)	6	15
All	All	740/800 (92%)	690 (93%)	50 (7%)	14	35

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LYS
2	B	178	SER
2	B	181	GLU
2	B	189	ILE
2	B	201	MET
2	B	237	ARG
2	B	243	LYS
2	B	283	LEU
2	B	306	ARG
2	B	375	CYS
2	B	376	SER
2	B	407	THR
2	B	423	VAL
1	D	88	LEU
1	D	89	SER
1	D	96	ARG
1	D	118	LEU
2	E	186	ASP
2	E	188	SER
2	E	194	ARG
2	E	211	GLU
2	E	243	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	283	LEU
2	E	303	ARG
2	E	304	LEU
2	E	306	ARG
2	E	375	CYS
2	E	407	THR
2	E	412	ARG
2	E	423	VAL
2	E	444	LEU
3	F	4	VAL
3	F	17	SER
3	F	18	LEU
3	F	46	GLN
3	F	50	VAL
3	F	66	VAL
3	F	67	ASP
3	F	75	VAL
3	F	88	ILE
3	F	91	ASN
3	F	93	ARG
3	G	4	VAL
3	G	6	ARG
3	G	17	SER
3	G	18	LEU
3	G	46	GLN
3	G	50	VAL
3	G	75	VAL
3	G	88	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	HIS
2	B	193	HIS
2	B	413	GLN
2	B	425	ASN
1	D	99	GLN
1	D	113	HIS
2	E	193	HIS
2	E	207	ASN
2	E	413	GLN
2	E	425	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	27	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](#)

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	$\# Z > 2$
5	PG4	D	201	-	12,12,12	0.23	0	11,11,11	0.18	0
4	EDO	E	502	-	3,3,3	0.69	0	2,2,2	0.13	0
4	EDO	E	501	-	3,3,3	0.56	0	2,2,2	0.26	0
4	EDO	B	501	-	3,3,3	0.54	0	2,2,2	0.31	0
4	EDO	B	502	-	3,3,3	0.50	0	2,2,2	0.37	0
4	EDO	A	201	-	3,3,3	0.55	0	2,2,2	0.33	0
5	PG4	B	503	-	12,12,12	0.43	0	11,11,11	0.38	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	PG4	D	201	-	-	4/10/10/10	-
4	EDO	E	502	-	-	0/1/1/1	-
4	EDO	E	501	-	-	1/1/1/1	-
4	EDO	B	501	-	-	1/1/1/1	-
4	EDO	B	502	-	-	0/1/1/1	-
4	EDO	A	201	-	-	0/1/1/1	-
5	PG4	B	503	-	-	7/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	201	PG4	O2-C3-C4-O3
5	B	503	PG4	O1-C1-C2-O2
5	B	503	PG4	O3-C5-C6-O4
5	D	201	PG4	O1-C1-C2-O2
5	B	503	PG4	O2-C3-C4-O3
5	D	201	PG4	C4-C3-O2-C2
5	B	503	PG4	C3-C4-O3-C5
5	D	201	PG4	C5-C6-O4-C7
5	B	503	PG4	C8-C7-O4-C6
4	B	501	EDO	O1-C1-C2-O2
5	B	503	PG4	C4-C3-O2-C2
4	E	501	EDO	O1-C1-C2-O2
5	B	503	PG4	C6-C5-O3-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	201	PG4	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	92/93 (98%)	0.08	5 (5%) 31 27	28, 45, 82, 98	0
1	D	93/93 (100%)	0.01	2 (2%) 62 59	26, 43, 64, 77	0
2	B	281/294 (95%)	-0.04	15 (5%) 32 28	24, 37, 69, 92	0
2	E	270/294 (91%)	-0.12	10 (3%) 45 41	25, 36, 66, 91	0
3	F	99/99 (100%)	0.22	3 (3%) 52 49	22, 45, 80, 89	0
3	G	96/99 (96%)	1.20	23 (23%) 2 1	24, 63, 93, 109	0
All	All	931/972 (95%)	0.11	58 (6%) 26 23	22, 40, 78, 109	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	11	VAL	5.5
2	E	163	PRO	5.4
3	G	27	HIS	5.3
3	G	26	SER	4.8
3	F	97	ASP	4.8
3	G	92	TYR	4.6
2	B	280	VAL	4.5
3	G	28	GLY	4.2
3	G	94	THR	3.8
2	B	281	GLY	3.8
2	B	164	PRO	3.7
3	G	9	GLU	3.7
1	D	60	THR	3.6
3	G	10	VAL	3.6
1	A	88	LEU	3.4
2	E	445	PRO	3.3
2	E	277	VAL	3.2
2	E	428	TRP	3.1
2	E	186	ASP	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	244	GLY	3.0
3	G	63	LYS	3.0
2	B	220	ALA	3.0
3	G	13	ALA	3.0
2	B	446	PRO	3.0
2	B	244	GLY	2.9
2	E	212	ASP	2.9
3	G	42	ASN	2.8
2	B	279	PRO	2.8
3	G	66	VAL	2.7
3	G	67	ASP	2.7
2	B	278	GLN	2.7
1	A	61	THR	2.7
2	B	219	GLN	2.6
3	F	42	ASN	2.5
2	B	246	SER	2.5
2	B	277	VAL	2.5
2	E	245	ALA	2.5
2	B	163	PRO	2.4
2	B	186	ASP	2.4
3	G	44	PRO	2.4
3	G	64	PRO	2.4
1	A	118	LEU	2.4
3	G	12	ALA	2.4
2	B	162	THR	2.3
2	E	162	THR	2.3
3	G	29	TYR	2.3
3	G	5	PRO	2.3
3	G	15	PRO	2.3
2	B	428	TRP	2.3
3	G	55	GLY	2.2
1	D	108	LEU	2.2
2	E	278	GLN	2.2
3	G	14	THR	2.1
1	A	87	HIS	2.1
3	F	67	ASP	2.1
1	A	89	SER	2.1
3	G	54	LYS	2.1
3	G	25	PRO	2.1

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($\text{\AA}^2$)	Q<0.9
4	EDO	A	201	4/4	0.81	0.21	65,65,65,65	0
4	EDO	E	502	4/4	0.81	0.19	61,64,64,65	0
5	PG4	D	201	13/13	0.81	0.16	72,74,85,85	0
5	PG4	B	503	13/13	0.83	0.16	49,55,61,62	0
4	EDO	B	502	4/4	0.89	0.13	50,50,52,52	0
4	EDO	E	501	4/4	0.91	0.10	47,47,47,47	0
4	EDO	B	501	4/4	0.92	0.14	59,60,60,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.