



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:28 PM UTC

PDB ID : 3QD6 / pdb_00003qd6
Title : Crystal structure of the CD40 and CD154 (CD40L) complex
Authors : Lee, J.-O.; Kim, Y.J.; Song, D.H.; Kim, H.M.; Park, B.S.
Deposited on : 2011-01-18
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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

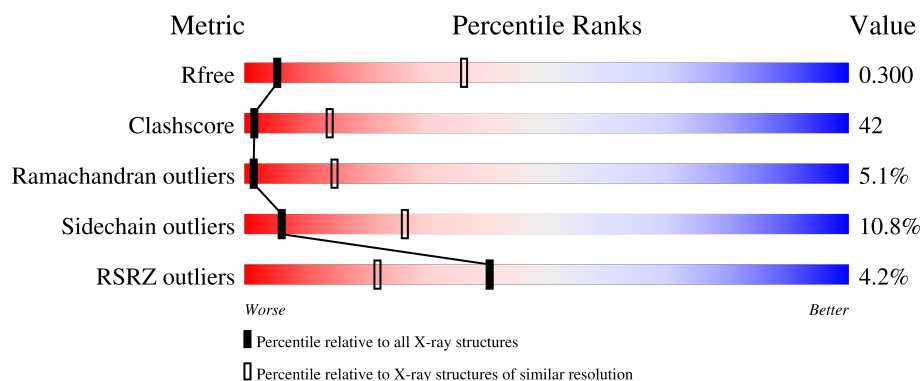
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	149	6% 42% 38% 9% 9%
1	B	149	5% 35% 46% 8% 9%
1	C	149	5% 40% 41% 9% 9%
1	D	149	% 38% 40% 12% 9%
1	E	149	% 43% 40% 7% 9%

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Mol	Chain	Length	Quality of chain
1	F	149	3% 40% 41% 10% 9%
2	R	177	3% 24% 32% 8% 36%
2	S	177	3% 27% 33% 7% 33%
2	T	177	3% 20% 34% 10% 36%
2	U	177	3% 31% 32% 33%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9896 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 CD40 ligand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	135	Total	C	N	O	S	0	0	0
			1033	658	178	193	4			
1	B	135	Total	C	N	O	S	0	0	0
			1033	658	178	193	4			
1	C	135	Total	C	N	O	S	0	0	0
			1033	658	178	193	4			
1	D	135	Total	C	N	O	S	0	0	0
			1033	658	178	193	4			
1	E	135	Total	C	N	O	S	0	0	0
			1033	658	178	193	4			
1	F	135	Total	C	N	O	S	0	0	0
			1033	658	178	193	4			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	ALA	-	expression tag	UNP P29965
A	114	ASP	-	expression tag	UNP P29965
A	115	PRO	-	expression tag	UNP P29965
B	113	ALA	-	expression tag	UNP P29965
B	114	ASP	-	expression tag	UNP P29965
B	115	PRO	-	expression tag	UNP P29965
C	113	ALA	-	expression tag	UNP P29965
C	114	ASP	-	expression tag	UNP P29965
C	115	PRO	-	expression tag	UNP P29965
D	113	ALA	-	expression tag	UNP P29965
D	114	ASP	-	expression tag	UNP P29965
D	115	PRO	-	expression tag	UNP P29965
E	113	ALA	-	expression tag	UNP P29965
E	114	ASP	-	expression tag	UNP P29965
E	115	PRO	-	expression tag	UNP P29965
F	113	ALA	-	expression tag	UNP P29965
F	114	ASP	-	expression tag	UNP P29965

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Chain	Residue	Modelled	Actual	Comment	Reference
F	115	PRO	-	expression tag	UNP P29965

- Molecule 2 is a protein called Tumor necrosis factor receptor superfamily member 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	114	Total	C	N	O	S	0	0	0
			886	532	154	184	16			
2	S	119	Total	C	N	O	S	0	0	0
			921	554	159	192	16			
2	T	114	Total	C	N	O	S	0	0	0
			886	532	154	184	16			
2	U	119	Total	C	N	O	S	0	0	0
			921	554	159	192	16			

There are 28 discrepancies between the modelled and reference sequences:

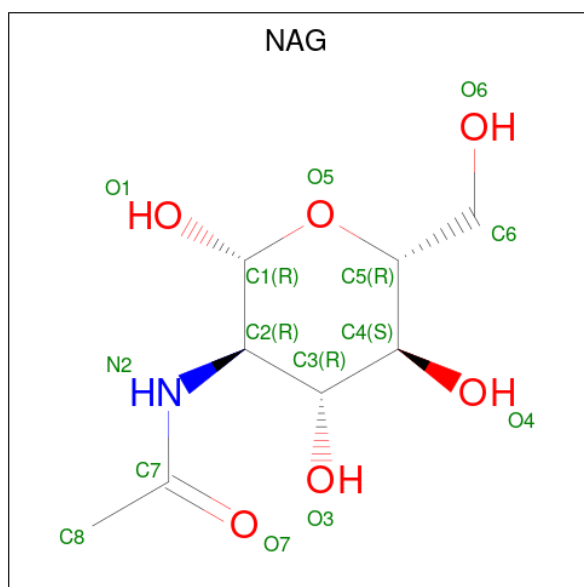
Chain	Residue	Modelled	Actual	Comment	Reference
R	191	SER	-	expression tag	UNP P25942
R	192	GLY	-	expression tag	UNP P25942
R	193	ARG	-	expression tag	UNP P25942
R	194	LEU	-	expression tag	UNP P25942
R	195	VAL	-	expression tag	UNP P25942
R	196	PRO	-	expression tag	UNP P25942
R	197	ARG	-	expression tag	UNP P25942
S	191	SER	-	expression tag	UNP P25942
S	192	GLY	-	expression tag	UNP P25942
S	193	ARG	-	expression tag	UNP P25942
S	194	LEU	-	expression tag	UNP P25942
S	195	VAL	-	expression tag	UNP P25942
S	196	PRO	-	expression tag	UNP P25942
S	197	ARG	-	expression tag	UNP P25942
T	191	SER	-	expression tag	UNP P25942
T	192	GLY	-	expression tag	UNP P25942
T	193	ARG	-	expression tag	UNP P25942
T	194	LEU	-	expression tag	UNP P25942
T	195	VAL	-	expression tag	UNP P25942
T	196	PRO	-	expression tag	UNP P25942
T	197	ARG	-	expression tag	UNP P25942
U	191	SER	-	expression tag	UNP P25942
U	192	GLY	-	expression tag	UNP P25942
U	193	ARG	-	expression tag	UNP P25942
U	194	LEU	-	expression tag	UNP P25942

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Chain	Residue	Modelled	Actual	Comment	Reference
U	195	VAL	-	expression tag	UNP P25942
U	196	PRO	-	expression tag	UNP P25942
U	197	ARG	-	expression tag	UNP P25942

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

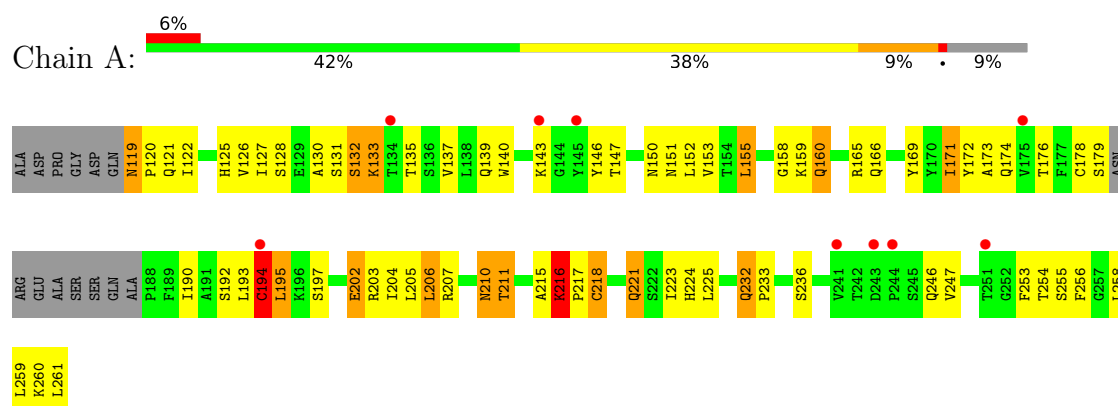


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		

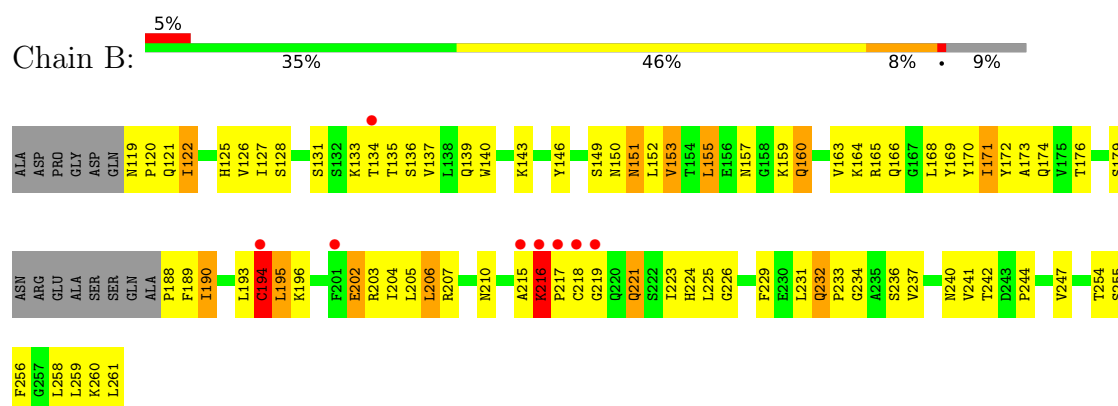
3 Residue-property plots [i](#)

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.

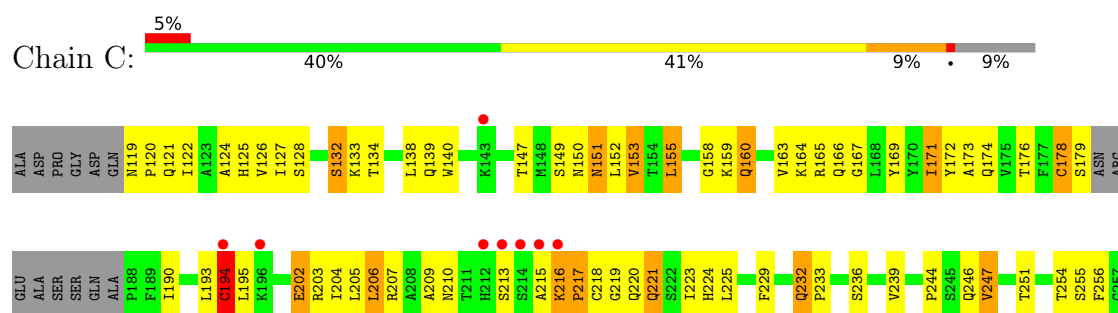
• Molecule 1: CD40 ligand



• Molecule 1: CD40 ligand



• Molecule 1: CD40 ligand



L258
L259
K260
L261

• Molecule 1: CD40 ligand



ALA ASP PRO GLN N119 P120 Q121 I122 H125 V126 I127 K133 T134 T135 S136 V137 L138 Q139 W140 K143 Y146 S149 N150 N151 L152 V153 L154 L155 L156 N157 G158 K159 Q160 L161 T162 V163 K164 R165 Q166 G167 L168 Y169 Y170 I171 Y172 A173 Q174 S179 ASN ARG GLU ALA

SER SER GLN P188 F189 I190 L193 C194 L195 K196 S197 F201 E202 R203 L204 L205 L206 R207 H212 A215 K216 C217 C218 G219 Q220 Q221 Q222 S222 H224 L225 G226 F229 Q232 P233 S236 V241 V244 P244 S245 Q246 Y247 G250 T254 S255 L258 L259 K260 L261

• Molecule 1: CD40 ligand



ALA ASP PRO GLN N119 P120 Q121 I122 H125 V126 I127 S128 S131 S132 K133 T134 T135 S136 Q139 W140 K143 Y146 Y148 S149 L223 L225 L226 V153 T154 L155 K159 Q160 K164 R165 Q166 Y169 Y170 I171 S179 ASN ARG GLU ALA SER SER GLU ALA

P188 F189 I190 L193 C194 L195 K196 S197 E202 R203 L204 L205 L206 R207 A208 S210 K210 T211 H212 A215 K216 C217 C218 G219 Q220 Q221 H224 L225 F229 S236 V237 F238 V239 P244 T254 S255 F256 G257 L258 L261

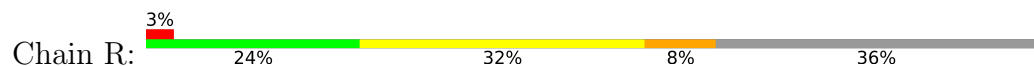
• Molecule 1: CD40 ligand



ALA ASP PRO GLN N119 P120 Q121 I122 A124 H125 V126 I127 S128 R203 L204 L205 S131 S132 K133 T134 Q139 W140 T147 M148 N149 N150 N151 L152 V153 T154 L155 E156 N157 G158 K159 Q160 L161 T162 V163 R165 Q166 G167 L168 Y169 Y170 I171 Y172 A173 Q174 C178 S179 ASN ARG GLU

ALA SER SER GLN P188 S192 L193 C194 L195 K196 S197 P198 E202 R203 L204 L205 L206 R207 N210 T211 H212 A215 K216 C217 C218 G219 Q220 Q221 S222 I223 H224 L225 V228 L231 Q232 P233 S236 V237 P244 Y247 T254 S255 F256 G257 L258 L259 K260 L261

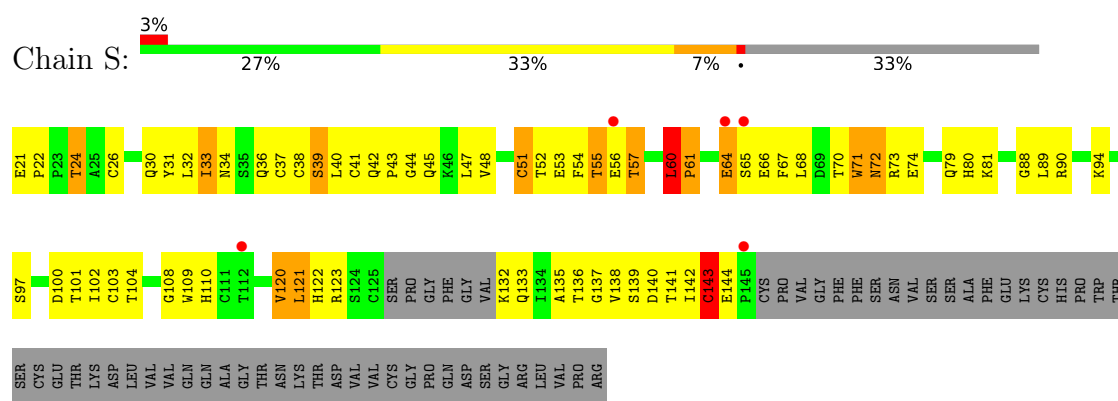
• Molecule 2: Tumor necrosis factor receptor superfamily member 5



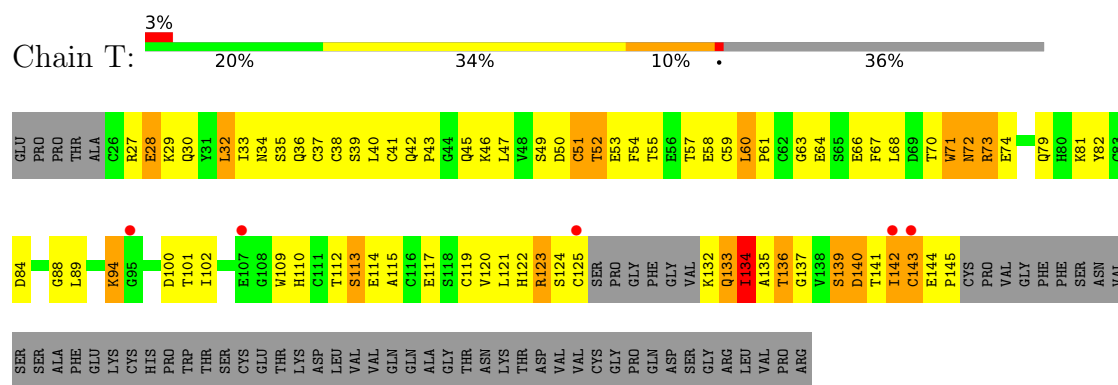
GLU PRO PRO THR C26 R27 E28 R29 Q30 Y31 L32 L33 N34 S35 C38 S39 L40 P43 G44 Q45 L46 L47 V48 S49 D50 C51 T52 E53 F54 T55 E56 T57 E58 C59 L60 G63 E64 S65 E66 F67 L68 D69 T70 W71 N72 R73 E74 C77 H78 S79 Q79 H80 K81 G88 L89

K94 S97 E98 T99 D100 T101 I102 G108 W109 H110 C111 T112 S113 E114 A115 C116 E117 S118 C119 V120 L121 H122 C125 SER PRO GLY PHE VAL K132 Q133 T134 A135 T136 G137 V138 S139 D140 T141 T142 C143 E144 CYS PRO VAL GLY PHE PHE SER ASN VAL SER SER ALA PHE

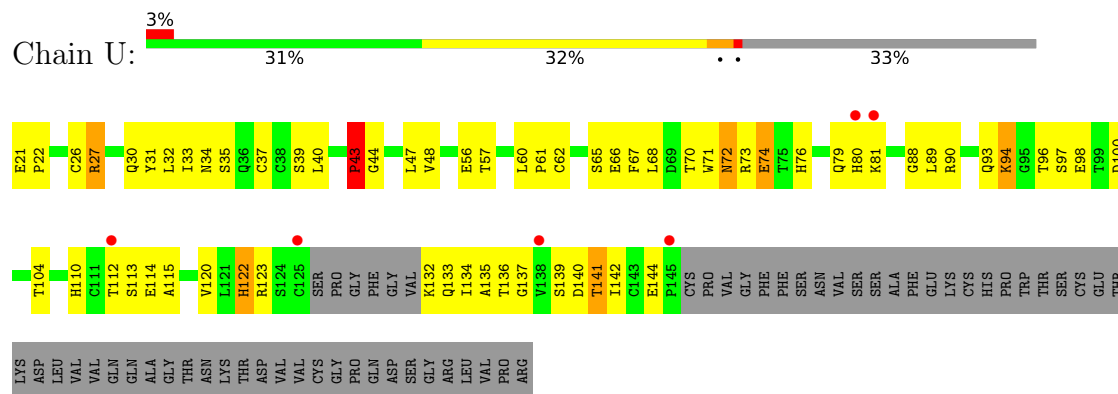
• Molecule 2: Tumor necrosis factor receptor superfamily member 5



• Molecule 2: Tumor necrosis factor receptor superfamily member 5



• Molecule 2: Tumor necrosis factor receptor superfamily member 5



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	133.21Å 133.21Å 211.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	114.96 – 3.50 114.96 – 3.50	Depositor EDS
% Data completeness (in resolution range)	92.9 (114.96-3.50) 92.9 (114.96-3.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 3.49Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.245 , 0.298 0.246 , 0.300	Depositor DCC
R_{free} test set	1209 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	76.1	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 96.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	9896	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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: NAG

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	0.70	1/1055 (0.1%)	1.02	5/1427 (0.4%)
1	B	0.67	2/1055 (0.2%)	0.98	4/1427 (0.3%)
1	C	0.63	1/1055 (0.1%)	0.97	3/1427 (0.2%)
1	D	0.66	1/1055 (0.1%)	0.99	3/1427 (0.2%)
1	E	0.61	0/1055	1.00	1/1427 (0.1%)
1	F	0.63	0/1055	0.94	0/1427
2	R	0.48	0/901	0.86	1/1218 (0.1%)
2	S	0.56	0/938	1.03	5/1271 (0.4%)
2	T	0.54	0/901	0.96	3/1218 (0.2%)
2	U	0.51	0/938	0.92	2/1271 (0.2%)
All	All	0.61	5/10008 (0.0%)	0.97	27/13540 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	194	CYS	CA-C	7.29	1.61	1.52
1	B	194	CYS	CA-C	6.44	1.60	1.52
1	D	194	CYS	CA-C	6.06	1.60	1.52
1	C	194	CYS	CA-C	5.12	1.59	1.52
1	B	194	CYS	CA-CB	5.02	1.61	1.53

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	60	LEU	CA-C-N	7.77	128.24	119.93
2	S	60	LEU	C-N-CA	7.77	128.24	119.93
2	U	73	ARG	N-CA-C	-7.56	102.13	112.03
2	R	73	ARG	N-CA-C	-7.18	102.63	112.03
2	S	143	CYS	N-CA-C	7.15	119.04	108.60

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	1033	0	1030	84	0
1	B	1033	0	1031	100	0
1	C	1033	0	1030	87	0
1	D	1033	0	1030	81	0
1	E	1033	0	1030	82	0
1	F	1033	0	1030	89	0
2	R	886	0	803	80	0
2	S	921	0	835	76	0
2	T	886	0	803	98	0
2	U	921	0	835	63	0
3	A	14	0	13	0	0
3	B	14	0	13	4	0
3	C	14	0	13	1	0
3	D	14	0	13	1	0
3	E	14	0	13	1	0
3	F	14	0	13	3	0
All	All	9896	0	9535	813	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 42.

The worst 5 of 813 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:T:136:THR:HG22	2:T:139:SER:HB2	1.25	1.16
1:D:259:LEU:HD22	1:E:261:LEU:HD21	1.27	1.15
1:B:171:ILE:HD11	1:B:193:LEU:HD11	1.32	1.11
1:E:166:GLN:HB2	1:E:233:PRO:HD3	1.32	1.11
1:E:216:LYS:HB2	1:E:217:PRO:HD3	1.28	1.08

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	131/149 (88%)	107 (82%)	18 (14%)	6 (5%)	2	17
1	B	131/149 (88%)	106 (81%)	21 (16%)	4 (3%)	3	25
1	C	131/149 (88%)	106 (81%)	22 (17%)	3 (2%)	5	30
1	D	131/149 (88%)	109 (83%)	16 (12%)	6 (5%)	2	17
1	E	131/149 (88%)	111 (85%)	16 (12%)	4 (3%)	3	25
1	F	131/149 (88%)	109 (83%)	13 (10%)	9 (7%)	1	10
2	R	110/177 (62%)	82 (74%)	16 (14%)	12 (11%)	0	5
2	S	115/177 (65%)	78 (68%)	34 (30%)	3 (3%)	4	27
2	T	110/177 (62%)	80 (73%)	20 (18%)	10 (9%)	0	7
2	U	115/177 (65%)	86 (75%)	23 (20%)	6 (5%)	1	14
All	All	1236/1602 (77%)	974 (79%)	199 (16%)	63 (5%)	1	15

5 of 63 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	SER
1	A	133	LYS
1	A	216	LYS
1	B	216	LYS
1	D	216	LYS

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	114/124 (92%)	98 (86%)	16 (14%)	3	19
1	B	114/124 (92%)	103 (90%)	11 (10%)	8	30
1	C	114/124 (92%)	102 (90%)	12 (10%)	6	27
1	D	114/124 (92%)	98 (86%)	16 (14%)	3	19
1	E	114/124 (92%)	102 (90%)	12 (10%)	6	27
1	F	114/124 (92%)	102 (90%)	12 (10%)	6	27
2	R	106/160 (66%)	98 (92%)	8 (8%)	12	37
2	S	110/160 (69%)	96 (87%)	14 (13%)	4	21
2	T	106/160 (66%)	94 (89%)	12 (11%)	5	25
2	U	110/160 (69%)	102 (93%)	8 (7%)	13	38
All	All	1116/1384 (81%)	995 (89%)	121 (11%)	6	26

5 of 121 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	153	VAL
2	T	134	ILE
1	F	155	LEU
2	T	133	GLN
2	U	72	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	119	ASN
2	R	80	HIS
2	U	110	HIS
2	U	30	GLN
1	F	139	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](#)

6 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	NAG	E	1411	1	14,14,15	0.92	1 (7%)	17,19,21	1.43	3 (17%)
3	NAG	D	1411	1	14,14,15	0.92	1 (7%)	17,19,21	0.77	1 (5%)
3	NAG	B	1411	1	14,14,15	0.82	1 (7%)	17,19,21	0.77	0
3	NAG	C	1411	1	14,14,15	0.77	0	17,19,21	0.92	1 (5%)
3	NAG	F	1411	1	14,14,15	1.07	1 (7%)	17,19,21	0.80	1 (5%)
3	NAG	A	1411	1	14,14,15	0.79	1 (7%)	17,19,21	0.99	1 (5%)

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
3	NAG	E	1411	1	-	4/6/23/26	0/1/1/1
3	NAG	D	1411	1	-	4/6/23/26	0/1/1/1
3	NAG	B	1411	1	-	4/6/23/26	0/1/1/1
3	NAG	C	1411	1	-	4/6/23/26	0/1/1/1
3	NAG	F	1411	1	-	5/6/23/26	0/1/1/1
3	NAG	A	1411	1	-	4/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1411	NAG	C1-C2	2.55	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1411	NAG	C1-C2	2.36	1.55	1.52
3	B	1411	NAG	C1-C2	2.22	1.55	1.52
3	D	1411	NAG	C1-C2	2.20	1.55	1.52
3	E	1411	NAG	C4-C5	2.09	1.57	1.53

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1411	NAG	C2-N2-C7	-2.90	119.01	122.90
3	E	1411	NAG	C4-C3-C2	-2.71	107.04	111.02
3	E	1411	NAG	C1-O5-C5	2.63	115.71	112.19
3	A	1411	NAG	C3-C4-C5	-2.18	106.28	110.23
3	C	1411	NAG	C3-C4-C5	2.13	114.10	110.23

There are no chirality outliers.

5 of 25 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1411	NAG	C3-C2-N2-C7
3	A	1411	NAG	C8-C7-N2-C2
3	A	1411	NAG	O7-C7-N2-C2
3	B	1411	NAG	C8-C7-N2-C2
3	B	1411	NAG	O7-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1411	NAG	1	0
3	D	1411	NAG	1	0
3	B	1411	NAG	4	0
3	C	1411	NAG	1	0
3	F	1411	NAG	3	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 [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	135/149 (90%)	0.43	9 (6%) 24 15	29, 58, 89, 97	0
1	B	135/149 (90%)	0.30	8 (5%) 28 16	29, 58, 84, 88	0
1	C	135/149 (90%)	0.42	8 (5%) 28 16	29, 59, 91, 99	0
1	D	135/149 (90%)	0.19	2 (1%) 72 47	27, 56, 79, 94	0
1	E	135/149 (90%)	0.25	2 (1%) 72 47	29, 59, 89, 98	0
1	F	135/149 (90%)	0.39	4 (2%) 52 30	29, 59, 91, 96	0
2	R	114/177 (64%)	0.27	5 (4%) 39 21	60, 88, 106, 112	0
2	S	119/177 (67%)	0.30	5 (4%) 40 22	41, 71, 110, 115	0
2	T	114/177 (64%)	0.43	5 (4%) 39 21	58, 79, 112, 119	0
2	U	119/177 (67%)	0.38	6 (5%) 34 19	43, 75, 101, 105	0
All	All	1276/1602 (79%)	0.33	54 (4%) 40 22	27, 65, 101, 119	0

The worst 5 of 54 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	213	SER	5.0
2	U	81	LYS	4.7
1	A	145	TYR	4.1
1	F	194	CYS	3.6
2	U	112	THR	3.4

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
3	NAG	E	1411	14/15	0.67	0.18	74,79,81,81	0
3	NAG	A	1411	14/15	0.68	0.15	78,82,86,87	0
3	NAG	F	1411	14/15	0.69	0.21	75,81,82,83	0
3	NAG	D	1411	14/15	0.71	0.20	84,89,92,92	0
3	NAG	C	1411	14/15	0.73	0.17	88,94,97,97	0
3	NAG	B	1411	14/15	0.77	0.14	81,84,86,86	0

6.5 Other polymers [i](#)

There are no such residues in this entry.