



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:33 AM UTC

PDB ID : 3EVX / pdb\_00003evx  
Title : Crystal structure of the human E2-like ubiquitin-fold modifier conjugating enzyme 1 (Ufc1). Northeast Structural Genomics Consortium target HR41  
Authors : Forouhar, F.; Abashidze, M.; Seetharaman, J.; Ho, C.K.; Janjua, H.; Cunningham, K.; Ma, L.-C.; Xiao, R.; Baran, M.C.; Acton, T.B.; Rost, B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)  
Deposited on : 2008-10-13  
Resolution : 2.54 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](mailto: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)

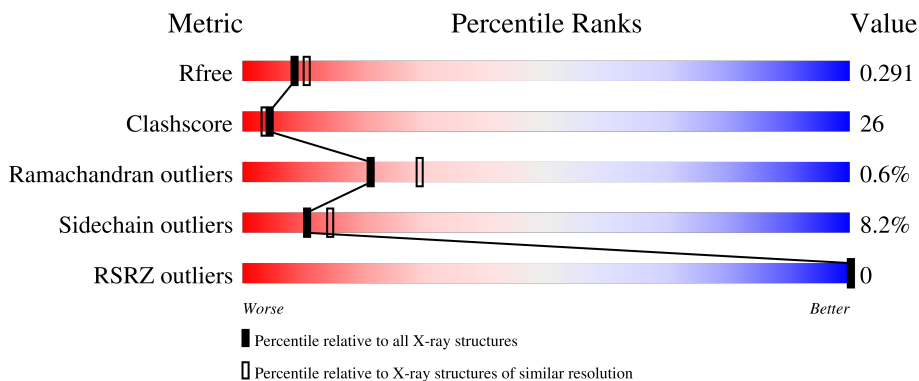
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.54 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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  $\geq 3$ , 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	175	
1	B	175	
1	C	175	
1	D	175	

Validation Pipeline (wwPDB-VP) : 2.49

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
2	SCN	D	176	-	-	X	-

## 2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 5389 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 Ufm1-conjugating enzyme 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	158	1302	844	226	228	2	2	0	0	0
1	B	158	1302	844	226	228	2	2	0	0	0
1	C	158	1302	844	226	228	2	2	0	0	0
1	D	158	1302	844	226	228	2	2	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

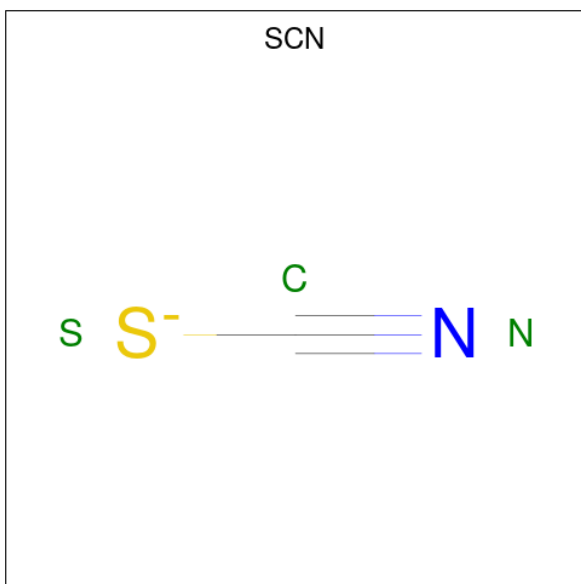
Chain	Residue	Modelled	Actual	Comment	Reference
A	168	LEU	-	expression tag	UNP Q9Y3C8
A	169	GLU	-	expression tag	UNP Q9Y3C8
A	170	HIS	-	expression tag	UNP Q9Y3C8
A	171	HIS	-	expression tag	UNP Q9Y3C8
A	172	HIS	-	expression tag	UNP Q9Y3C8
A	173	HIS	-	expression tag	UNP Q9Y3C8
A	174	HIS	-	expression tag	UNP Q9Y3C8
A	175	HIS	-	expression tag	UNP Q9Y3C8
B	168	LEU	-	expression tag	UNP Q9Y3C8
B	169	GLU	-	expression tag	UNP Q9Y3C8
B	170	HIS	-	expression tag	UNP Q9Y3C8
B	171	HIS	-	expression tag	UNP Q9Y3C8
B	172	HIS	-	expression tag	UNP Q9Y3C8
B	173	HIS	-	expression tag	UNP Q9Y3C8
B	174	HIS	-	expression tag	UNP Q9Y3C8
B	175	HIS	-	expression tag	UNP Q9Y3C8
C	168	LEU	-	expression tag	UNP Q9Y3C8
C	169	GLU	-	expression tag	UNP Q9Y3C8
C	170	HIS	-	expression tag	UNP Q9Y3C8
C	171	HIS	-	expression tag	UNP Q9Y3C8
C	172	HIS	-	expression tag	UNP Q9Y3C8

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	173	HIS	-	expression tag	UNP Q9Y3C8
C	174	HIS	-	expression tag	UNP Q9Y3C8
C	175	HIS	-	expression tag	UNP Q9Y3C8
D	168	LEU	-	expression tag	UNP Q9Y3C8
D	169	GLU	-	expression tag	UNP Q9Y3C8
D	170	HIS	-	expression tag	UNP Q9Y3C8
D	171	HIS	-	expression tag	UNP Q9Y3C8
D	172	HIS	-	expression tag	UNP Q9Y3C8
D	173	HIS	-	expression tag	UNP Q9Y3C8
D	174	HIS	-	expression tag	UNP Q9Y3C8
D	175	HIS	-	expression tag	UNP Q9Y3C8

- Molecule 2 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	S	0	0
			3	1	1	1		
2	B	1	Total	C	N	S	0	0
			3	1	1	1		
2	C	1	Total	C	N	S	0	0
			3	1	1	1		
2	D	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 3 is water.

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	A	45	Total 45	O 45	0	0
3	B	40	Total 40	O 40	0	0
3	C	35	Total 35	O 35	0	0
3	D	49	Total 49	O 49	0	0





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	41.37Å 64.54Å 66.42Å 90.06° 89.95° 105.18°	Depositor
Resolution (Å)	19.96 – 2.54 19.96 – 2.54	Depositor EDS
% Data completeness (in resolution range)	91.0 (19.96-2.54) 95.8 (19.96-2.54)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.10 (at 2.45Å)	Xtrriage
Refinement program	CNS 1.2 & XtalView	Depositor
R, $R_{free}$	0.233 , 0.279 0.244 , 0.291	Depositor DCC
$R_{free}$ test set	2394 reflections (10.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.7	Xtrriage
Anisotropy	1.028	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 34.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.448 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5389	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 25.81 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9599e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: SCN

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	0.52	0/1337	0.90	3/1811 (0.2%)
1	B	0.51	0/1337	0.90	3/1811 (0.2%)
1	C	0.51	0/1337	0.90	4/1811 (0.2%)
1	D	0.51	0/1337	0.90	3/1811 (0.2%)
All	All	0.51	0/5348	0.90	13/7244 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	149	GLU	N-CA-C	7.50	119.24	111.14
1	A	149	GLU	N-CA-C	7.36	119.09	111.14
1	B	149	GLU	N-CA-C	7.12	118.83	111.14
1	C	149	GLU	N-CA-C	7.04	118.74	111.14
1	A	99	VAL	CA-C-N	5.95	127.28	119.84
1	A	99	VAL	C-N-CA	5.95	127.28	119.84
1	D	99	VAL	CA-C-N	5.90	127.22	119.84
1	D	99	VAL	C-N-CA	5.90	127.22	119.84
1	B	99	VAL	CA-C-N	5.76	127.04	119.84
1	B	99	VAL	C-N-CA	5.76	127.04	119.84
1	C	99	VAL	CA-C-N	5.72	126.99	119.84
1	C	99	VAL	C-N-CA	5.72	126.99	119.84
1	C	60	LYS	N-CA-C	5.11	117.24	111.11

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	1302	0	1303	74	0
1	B	1302	0	1303	70	0
1	C	1302	0	1303	74	0
1	D	1302	0	1303	74	0
2	A	3	0	0	1	0
2	B	3	0	0	0	0
2	C	3	0	0	1	0
2	D	3	0	0	2	0
3	A	45	0	0	6	0
3	B	40	0	0	6	0
3	C	35	0	0	9	0
3	D	49	0	0	11	0
All	All	5389	0	5212	275	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 26.

All (275) 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:D:28:TRP:HA	3:D:218:HOH:O	1.65	0.96
1:A:74:ASP:HA	1:D:155:GLN:HE21	1.36	0.90
1:A:155:GLN:HE21	1:D:74:ASP:HA	1.38	0.89
1:C:7:ARG:HD2	1:C:8:ARG:HH12	1.43	0.83
1:B:7:ARG:HD2	1:B:8:ARG:HH12	1.44	0.82
1:A:7:ARG:HD2	1:A:8:ARG:HH12	1.43	0.82
1:C:16:LEU:HD12	1:C:34:GLU:HB3	1.63	0.81
1:A:16:LEU:HD12	1:A:34:GLU:HB3	1.62	0.80
1:B:23:ARG:HH22	1:C:119:ASP:HB3	1.46	0.80
1:D:7:ARG:HD2	1:D:8:ARG:HH12	1.45	0.79
1:A:102:LEU:O	1:A:109:MSE:HE1	1.83	0.79
1:D:16:LEU:HD12	1:D:34:GLU:HB3	1.65	0.79
1:C:102:LEU:O	1:C:109:MSE:HE1	1.84	0.78
1:D:102:LEU:O	1:D:109:MSE:HE1	1.83	0.78
1:B:16:LEU:HD12	1:B:34:GLU:HB3	1.66	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:LEU:O	1:B:109:MSE:HE1	1.84	0.78
1:D:97:ILE:HG21	1:D:142:LEU:HG	1.67	0.77
1:A:97:ILE:HG21	1:A:142:LEU:HG	1.67	0.76
1:B:97:ILE:HG21	1:B:142:LEU:HG	1.68	0.74
1:C:97:ILE:HG21	1:C:142:LEU:HG	1.68	0.74
1:B:119:ASP:HB3	1:C:23:ARG:HH22	1.52	0.73
1:C:57:GLU:HG2	3:C:211:HOH:O	1.89	0.72
1:C:63:THR:OG1	1:C:64:ARG:HD2	1.90	0.72
1:D:63:THR:OG1	1:D:64:ARG:HD2	1.90	0.70
1:A:74:ASP:HA	1:D:155:GLN:NE2	2.06	0.70
1:A:155:GLN:NE2	1:D:74:ASP:HA	2.07	0.69
1:B:63:THR:OG1	1:B:64:ARG:HD2	1.92	0.69
1:D:28:TRP:HE3	3:D:218:HOH:O	1.76	0.68
1:A:63:THR:OG1	1:A:64:ARG:HD2	1.93	0.67
1:B:23:ARG:NH2	1:C:119:ASP:HB3	2.10	0.66
1:A:32:LEU:HG	1:A:36:TYR:CE2	2.31	0.66
1:C:56:LEU:HD22	1:C:138:MSE:HE3	1.78	0.66
1:A:57:GLU:HG2	3:A:217:HOH:O	1.95	0.65
1:C:111:ARG:HA	3:C:190:HOH:O	1.95	0.65
1:D:32:LEU:HG	1:D:36:TYR:CE2	2.31	0.65
1:B:32:LEU:HG	1:B:36:TYR:CE2	2.32	0.65
1:C:95:PRO:HD2	1:C:137:LEU:HD22	1.79	0.65
1:A:56:LEU:HD22	1:A:138:MSE:HE3	1.78	0.65
1:B:56:LEU:HD22	1:B:138:MSE:HE3	1.79	0.64
1:A:95:PRO:HD2	1:A:137:LEU:HD22	1.79	0.64
1:B:95:PRO:HD2	1:B:137:LEU:HD22	1.79	0.64
1:C:32:LEU:HG	1:C:36:TYR:CE2	2.32	0.64
1:D:56:LEU:HD22	1:D:138:MSE:HE3	1.78	0.63
1:A:68:LYS:NZ	1:A:68:LYS:HB3	2.13	0.63
1:D:95:PRO:HD2	1:D:137:LEU:HD22	1.79	0.62
1:B:119:ASP:HB3	1:C:23:ARG:NH2	2.14	0.62
1:A:101:GLU:HG3	3:A:177:HOH:O	1.99	0.62
1:B:5:ALA:HB1	3:B:183:HOH:O	2.00	0.61
1:A:83:GLU:OE2	1:A:100:PRO:HG2	2.00	0.60
1:A:100:PRO:HB2	3:A:215:HOH:O	2.00	0.60
1:C:61:GLU:HG3	3:C:191:HOH:O	2.01	0.60
1:C:83:GLU:OE2	1:C:100:PRO:HG2	2.01	0.60
1:B:83:GLU:OE2	1:B:100:PRO:HG2	2.02	0.59
1:A:5:ALA:HB1	3:A:207:HOH:O	2.02	0.59
1:D:68:LYS:NZ	1:D:68:LYS:HB3	2.16	0.59
1:A:159:ILE:C	1:A:159:ILE:HD13	2.28	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LYS:HD3	1:A:79:GLU:OE1	2.02	0.59
1:B:159:ILE:HD13	1:B:159:ILE:C	2.28	0.59
1:C:68:LYS:NZ	1:C:68:LYS:HB3	2.17	0.59
1:D:20:ALA:CB	3:D:218:HOH:O	2.51	0.59
1:C:159:ILE:C	1:C:159:ILE:HD13	2.28	0.58
1:B:25:ARG:HB3	2:D:176:SCN:S	2.44	0.58
1:B:68:LYS:NZ	1:B:68:LYS:HB3	2.19	0.58
1:D:159:ILE:C	1:D:159:ILE:HD13	2.28	0.58
1:C:68:LYS:HD3	1:C:79:GLU:OE1	2.04	0.57
1:D:83:GLU:OE2	1:D:100:PRO:HG2	2.04	0.57
1:C:90:TYR:CD1	1:C:91:PRO:HA	2.40	0.57
1:B:68:LYS:HD3	1:B:79:GLU:OE1	2.05	0.57
1:D:57:GLU:HG2	3:D:186:HOH:O	2.04	0.57
1:A:90:TYR:CD1	1:A:91:PRO:HA	2.39	0.57
1:A:72:ILE:HA	1:A:76:LEU:O	2.06	0.56
1:B:90:TYR:CD1	1:B:91:PRO:HA	2.40	0.56
1:D:68:LYS:HD3	1:D:79:GLU:OE1	2.05	0.56
1:A:78:TYR:CE1	1:A:161:HIS:HB2	2.41	0.56
1:C:5:ALA:HB1	3:C:202:HOH:O	2.05	0.56
1:C:117:LEU:HD22	1:C:117:LEU:H	1.71	0.56
1:A:111:ARG:NH1	1:B:48:ASN:HA	2.21	0.56
1:D:90:TYR:CD1	1:D:91:PRO:HA	2.40	0.56
1:C:111:ARG:NH1	1:D:48:ASN:HA	2.22	0.55
1:B:117:LEU:H	1:B:117:LEU:HD22	1.72	0.55
1:B:61:GLU:HG3	3:B:207:HOH:O	2.06	0.55
1:B:78:TYR:CE1	1:B:161:HIS:HB2	2.41	0.55
1:A:59:ASN:ND2	1:A:64:ARG:HD3	2.22	0.55
1:D:59:ASN:ND2	1:D:64:ARG:HD3	2.22	0.55
1:C:78:TYR:CE1	1:C:161:HIS:HB2	2.42	0.55
1:C:41:ARG:HH11	1:C:41:ARG:HG2	1.72	0.54
1:A:58:SER:HB3	1:A:65:TRP:CE3	2.42	0.54
1:D:72:ILE:HA	1:D:76:LEU:O	2.07	0.54
1:B:17:LYS:HG2	3:B:193:HOH:O	2.05	0.54
1:B:72:ILE:HA	1:B:76:LEU:O	2.07	0.54
1:C:72:ILE:HA	1:C:76:LEU:O	2.07	0.54
1:C:90:TYR:CG	1:C:91:PRO:HA	2.43	0.54
1:A:117:LEU:HD22	1:A:117:LEU:H	1.71	0.54
1:B:59:ASN:ND2	1:B:64:ARG:HD3	2.23	0.54
1:D:142:LEU:HD22	1:D:146:LEU:HG	1.90	0.54
1:B:68:LYS:HB3	1:B:68:LYS:HZ3	1.73	0.54
1:C:59:ASN:ND2	1:C:64:ARG:HD3	2.23	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:LEU:H	1:D:117:LEU:HD22	1.72	0.54
1:B:23:ARG:NH2	3:B:201:HOH:O	2.41	0.53
1:B:58:SER:HB3	1:B:65:TRP:CE3	2.43	0.53
1:B:142:LEU:HD22	1:B:146:LEU:HG	1.90	0.53
1:D:78:TYR:CE1	1:D:161:HIS:HB2	2.43	0.53
1:A:90:TYR:CG	1:A:91:PRO:HA	2.43	0.53
1:A:142:LEU:HD22	1:A:146:LEU:HG	1.91	0.53
1:C:106:THR:HB	1:C:153:LEU:HD21	1.91	0.53
1:D:90:TYR:CG	1:D:91:PRO:HA	2.43	0.53
1:D:41:ARG:HG2	1:D:41:ARG:HH11	1.74	0.53
1:B:90:TYR:CG	1:B:91:PRO:HA	2.43	0.53
1:D:58:SER:HB3	1:D:65:TRP:CE3	2.42	0.53
1:A:18:THR:N	3:A:186:HOH:O	2.40	0.53
1:B:106:THR:HB	1:B:153:LEU:HD21	1.91	0.53
1:D:47:LYS:CE	3:D:201:HOH:O	2.57	0.53
1:A:22:PRO:HA	1:A:28:TRP:CD2	2.44	0.52
1:A:106:THR:HB	1:A:153:LEU:HD21	1.91	0.52
1:C:104:GLY:HA2	1:D:44:GLU:OE1	2.09	0.52
1:C:39:LEU:O	1:C:43:VAL:HG23	2.10	0.52
1:C:111:ARG:HD2	3:C:190:HOH:O	2.10	0.52
1:C:142:LEU:HD22	1:C:146:LEU:HG	1.91	0.52
1:A:104:GLY:HA2	1:B:44:GLU:OE1	2.09	0.52
1:A:41:ARG:HG2	1:A:41:ARG:HH11	1.75	0.52
1:B:159:ILE:HD13	1:B:160:GLN:N	2.25	0.52
1:C:22:PRO:HA	1:C:28:TRP:CD2	2.45	0.52
1:C:58:SER:HB3	1:C:65:TRP:CE3	2.44	0.52
1:D:159:ILE:HD13	1:D:160:GLN:N	2.25	0.51
1:A:37:GLN:O	1:A:40:ILE:HG13	2.10	0.51
1:B:41:ARG:HG2	1:B:41:ARG:HH11	1.75	0.51
1:C:68:LYS:HB3	1:C:68:LYS:HZ3	1.75	0.51
1:C:127:ARG:NH2	3:C:193:HOH:O	2.44	0.51
1:B:16:LEU:N	1:B:16:LEU:HD22	2.26	0.51
1:C:21:GLY:C	1:C:23:ARG:H	2.19	0.51
1:D:106:THR:HB	1:D:153:LEU:HD21	1.91	0.51
1:D:122:LYS:HB3	1:D:123:PRO:HD3	1.92	0.51
1:B:22:PRO:HA	1:B:28:TRP:CD2	2.46	0.51
1:C:18:THR:OG1	1:C:34:GLU:OE2	2.24	0.51
1:C:37:GLN:O	1:C:40:ILE:HG13	2.10	0.51
1:A:32:LEU:HG	1:A:36:TYR:HE2	1.77	0.50
1:A:21:GLY:C	1:A:23:ARG:H	2.19	0.50
1:A:17:LYS:C	3:A:186:HOH:O	2.54	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:LEU:O	1:A:43:VAL:HG23	2.11	0.50
1:C:8:ARG:HA	1:C:8:ARG:NE	2.27	0.50
1:A:7:ARG:HD2	1:A:8:ARG:NH1	2.21	0.50
1:B:122:LYS:HB3	1:B:123:PRO:HD3	1.93	0.50
1:A:117:LEU:HD22	1:A:117:LEU:N	2.27	0.50
1:A:159:ILE:HD13	1:A:160:GLN:N	2.27	0.50
1:B:19:ASN:HD22	1:B:19:ASN:C	2.20	0.49
1:B:20:ALA:O	1:B:91:PRO:HD3	2.12	0.49
1:B:21:GLY:C	1:B:23:ARG:H	2.20	0.49
1:C:117:LEU:HD22	1:C:117:LEU:N	2.27	0.49
1:C:122:LYS:HB3	1:C:123:PRO:HD3	1.93	0.49
1:B:29:VAL:HG21	1:D:76:LEU:HD23	1.93	0.49
1:B:117:LEU:HD22	1:B:117:LEU:N	2.27	0.49
1:A:19:ASN:C	1:A:19:ASN:HD22	2.20	0.49
1:D:22:PRO:HA	1:D:28:TRP:CD2	2.47	0.49
1:B:8:ARG:HA	1:B:8:ARG:NE	2.28	0.49
1:B:115:ILE:HG23	1:B:145:TRP:CD1	2.48	0.49
1:C:19:ASN:C	1:C:19:ASN:HD22	2.20	0.49
1:C:76:LEU:HD23	2:C:176:SCN:N	2.28	0.49
1:D:16:LEU:N	1:D:16:LEU:HD22	2.28	0.49
1:C:99:VAL:HG11	1:C:102:LEU:HD12	1.95	0.49
1:D:8:ARG:HA	1:D:8:ARG:NE	2.27	0.49
1:D:32:LEU:HG	1:D:36:TYR:HE2	1.77	0.49
1:D:21:GLY:C	1:D:23:ARG:H	2.21	0.49
1:B:37:GLN:O	1:B:40:ILE:HG13	2.12	0.48
1:C:159:ILE:HD13	1:C:160:GLN:N	2.28	0.48
1:D:37:GLN:O	1:D:40:ILE:HG13	2.12	0.48
1:D:101:GLU:HG3	3:D:182:HOH:O	2.12	0.48
1:A:16:LEU:N	1:A:16:LEU:HD22	2.29	0.48
1:C:154:ILE:HG12	1:C:159:ILE:HG23	1.96	0.48
1:D:117:LEU:HD22	1:D:117:LEU:N	2.28	0.48
1:B:115:ILE:HD12	1:B:145:TRP:CE2	2.49	0.48
1:D:19:ASN:C	1:D:19:ASN:HD22	2.21	0.48
1:A:122:LYS:HB3	1:A:123:PRO:HD3	1.94	0.48
1:C:101:GLU:HG3	3:C:179:HOH:O	2.13	0.48
1:A:20:ALA:O	1:A:91:PRO:HD3	2.14	0.48
1:C:115:ILE:HD12	1:C:145:TRP:CE2	2.49	0.48
1:C:115:ILE:HG22	1:C:116:CYS:N	2.29	0.48
1:D:115:ILE:HG23	1:D:145:TRP:CD1	2.49	0.48
1:A:8:ARG:NE	1:A:8:ARG:HA	2.28	0.48
1:A:115:ILE:HG23	1:A:145:TRP:CD1	2.49	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ILE:HG12	1:A:159:ILE:HG23	1.95	0.47
1:D:17:LYS:HG2	3:D:202:HOH:O	2.14	0.47
1:B:39:LEU:O	1:B:43:VAL:HG23	2.13	0.47
1:D:69:CYS:SG	1:D:146:LEU:HD11	2.54	0.47
1:C:16:LEU:HD22	1:C:16:LEU:N	2.30	0.47
1:C:115:ILE:HG23	1:C:145:TRP:CD1	2.50	0.47
1:D:39:LEU:O	1:D:43:VAL:HG23	2.14	0.47
1:D:115:ILE:HD12	1:D:145:TRP:CE2	2.49	0.47
1:A:104:GLY:HA2	1:B:44:GLU:CD	2.39	0.47
1:B:99:VAL:HG11	1:B:102:LEU:HD12	1.97	0.47
1:C:104:GLY:HA2	1:D:44:GLU:CD	2.39	0.47
1:C:82:ILE:HG21	1:C:142:LEU:HD11	1.97	0.47
1:B:18:THR:O	1:B:31:ARG:HD3	2.15	0.47
1:B:58:SER:HB3	1:B:65:TRP:CD2	2.50	0.47
1:D:7:ARG:HD2	1:D:8:ARG:NH1	2.23	0.47
1:D:18:THR:O	1:D:31:ARG:HD3	2.15	0.47
1:D:76:LEU:HD23	2:D:176:SCN:N	2.30	0.47
1:C:20:ALA:O	1:C:91:PRO:HD3	2.15	0.47
1:A:115:ILE:HD12	1:A:145:TRP:CE2	2.49	0.46
1:A:115:ILE:HG22	1:A:116:CYS:N	2.29	0.46
1:D:102:LEU:C	1:D:109:MSE:HE1	2.41	0.46
1:A:18:THR:O	1:A:31:ARG:HD3	2.16	0.46
1:A:99:VAL:HG11	1:A:102:LEU:HD12	1.97	0.46
1:D:58:SER:HB3	1:D:65:TRP:CD2	2.51	0.46
1:B:154:ILE:HG12	1:B:159:ILE:HG23	1.98	0.46
1:C:18:THR:O	1:C:31:ARG:HD3	2.15	0.46
1:D:20:ALA:O	1:D:91:PRO:HD3	2.15	0.46
1:D:64:ARG:HB3	3:D:224:HOH:O	2.16	0.46
1:B:115:ILE:HG22	1:B:116:CYS:N	2.30	0.46
1:C:58:SER:HB3	1:C:65:TRP:CD2	2.52	0.45
1:D:115:ILE:HG22	1:D:116:CYS:N	2.30	0.45
1:D:99:VAL:HG11	1:D:102:LEU:HD12	1.98	0.45
1:A:102:LEU:C	1:A:109:MSE:HE1	2.41	0.45
1:D:154:ILE:HG12	1:D:159:ILE:HG23	1.98	0.45
1:D:68:LYS:HB3	1:D:68:LYS:HZ3	1.79	0.45
1:A:76:LEU:HD23	2:A:176:SCN:N	2.32	0.45
1:A:82:ILE:HG21	1:A:142:LEU:HD11	1.98	0.45
1:B:69:CYS:SG	1:B:146:LEU:HD11	2.57	0.45
1:C:102:LEU:C	1:C:109:MSE:HE1	2.41	0.44
1:A:58:SER:HB3	1:A:65:TRP:CD2	2.52	0.44
1:D:96:GLU:HB3	1:D:114:LYS:HD2	2.00	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:GLU:HB3	1:A:114:LYS:HD2	2.00	0.44
1:A:69:CYS:SG	1:A:146:LEU:HD11	2.58	0.44
1:B:82:ILE:HG21	1:B:142:LEU:HD11	1.99	0.43
1:B:102:LEU:C	1:B:109:MSE:HE1	2.41	0.43
1:C:146:LEU:O	1:C:150:ILE:HG12	2.18	0.43
1:B:96:GLU:HB3	1:B:114:LYS:HD2	2.00	0.43
1:D:20:ALA:HB3	3:D:218:HOH:O	2.14	0.43
1:C:96:GLU:HB3	1:C:114:LYS:HD2	2.00	0.43
1:D:146:LEU:O	1:D:150:ILE:HG12	2.19	0.43
1:A:68:LYS:HB3	1:A:68:LYS:HZ2	1.83	0.43
1:A:146:LEU:O	1:A:150:ILE:HG12	2.19	0.43
1:B:101:GLU:HG3	3:B:179:HOH:O	2.17	0.43
1:B:152:ASP:OD1	1:B:156:LYS:HE3	2.19	0.43
1:C:97:ILE:HD11	1:C:137:LEU:HG	2.01	0.43
1:D:82:ILE:HG21	1:D:142:LEU:HD11	1.99	0.42
1:C:32:LEU:HG	1:C:36:TYR:HE2	1.79	0.42
1:B:8:ARG:HG2	3:B:206:HOH:O	2.18	0.42
1:B:146:LEU:O	1:B:150:ILE:HG12	2.19	0.42
1:A:78:TYR:CZ	1:A:161:HIS:HB2	2.55	0.42
1:D:97:ILE:HD11	1:D:137:LEU:HG	2.00	0.42
1:B:23:ARG:HH12	1:C:119:ASP:CG	2.26	0.42
1:D:51:ASN:O	1:D:53:TRP:HD1	2.02	0.42
1:B:32:LEU:HG	1:B:36:TYR:HE2	1.79	0.41
1:B:97:ILE:HD11	1:B:137:LEU:HG	2.01	0.41
1:C:121:PHE:O	1:C:122:LYS:C	2.63	0.41
1:D:152:ASP:OD1	1:D:156:LYS:HE3	2.21	0.41
1:C:23:ARG:HD3	3:C:198:HOH:O	2.20	0.41
1:A:7:ARG:HB3	1:A:8:ARG:NH1	2.35	0.41
1:A:51:ASN:O	1:A:53:TRP:HD1	2.04	0.41
1:A:121:PHE:O	1:A:122:LYS:C	2.64	0.41
1:C:7:ARG:HB3	1:C:8:ARG:NH1	2.35	0.41
1:C:69:CYS:SG	1:C:146:LEU:HD11	2.61	0.41
1:D:110:TYR:CD1	1:D:116:CYS:HB3	2.56	0.41
1:D:129:VAL:HA	1:D:130:PRO:HA	1.84	0.41
1:A:103:ASP:HA	1:A:109:MSE:HE3	2.02	0.41
1:B:119:ASP:CG	1:C:23:ARG:HH12	2.28	0.41
1:C:115:ILE:CG2	1:C:116:CYS:N	2.84	0.41
1:C:103:ASP:HA	1:C:109:MSE:HE3	2.03	0.41
1:C:114:LYS:NZ	3:C:209:HOH:O	2.53	0.41
1:A:41:ARG:HA	1:A:41:ARG:NH1	2.36	0.41
1:D:160:GLN:HB3	3:D:223:HOH:O	2.21	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ARG:HH21	1:A:23:ARG:HG2	1.86	0.41
1:A:110:TYR:CD1	1:A:116:CYS:HB3	2.56	0.41
1:B:78:TYR:CZ	1:B:161:HIS:HB2	2.56	0.41
1:B:103:ASP:HA	1:B:109:MSE:HE3	2.03	0.41
1:A:68:LYS:HB3	1:A:68:LYS:HZ3	1.83	0.41
1:A:115:ILE:CG2	1:A:116:CYS:N	2.84	0.41
1:D:47:LYS:HE2	3:D:201:HOH:O	2.17	0.41
1:A:152:ASP:OD1	1:A:156:LYS:HE3	2.21	0.40
1:B:51:ASN:O	1:B:53:TRP:HD1	2.04	0.40
1:B:110:TYR:CD1	1:B:116:CYS:HB3	2.56	0.40
1:A:97:ILE:HD11	1:A:137:LEU:HG	2.02	0.40
1:C:21:GLY:O	1:C:23:ARG:N	2.54	0.40
1:D:18:THR:OG1	1:D:34:GLU:OE2	2.27	0.40
1:C:51:ASN:O	1:C:53:TRP:HD1	2.04	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	156/175 (89%)	145 (93%)	10 (6%)	1 (1%)	21	29
1	B	156/175 (89%)	145 (93%)	10 (6%)	1 (1%)	21	29
1	C	156/175 (89%)	145 (93%)	10 (6%)	1 (1%)	21	29
1	D	156/175 (89%)	145 (93%)	10 (6%)	1 (1%)	21	29
All	All	624/700 (89%)	580 (93%)	40 (6%)	4 (1%)	21	29

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	22	PRO

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	22	PRO
1	A	22	PRO
1	D	22	PRO

### 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	138/151 (91%)	127 (92%)	11 (8%)	11	15
1	B	138/151 (91%)	126 (91%)	12 (9%)	9	13
1	C	138/151 (91%)	127 (92%)	11 (8%)	11	15
1	D	138/151 (91%)	127 (92%)	11 (8%)	11	15
All	All	552/604 (91%)	507 (92%)	45 (8%)	10	14

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ARG
1	A	17	LYS
1	A	19	ASN
1	A	41	ARG
1	A	68	LYS
1	A	100	PRO
1	A	106	THR
1	A	118	THR
1	A	119	ASP
1	A	142	LEU
1	A	159	ILE
1	B	8	ARG
1	B	17	LYS
1	B	19	ASN
1	B	41	ARG
1	B	68	LYS
1	B	100	PRO
1	B	106	THR

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	118	THR
1	B	119	ASP
1	B	130	PRO
1	B	142	LEU
1	B	159	ILE
1	C	8	ARG
1	C	17	LYS
1	C	19	ASN
1	C	41	ARG
1	C	68	LYS
1	C	100	PRO
1	C	106	THR
1	C	118	THR
1	C	119	ASP
1	C	142	LEU
1	C	159	ILE
1	D	8	ARG
1	D	17	LYS
1	D	19	ASN
1	D	41	ARG
1	D	68	LYS
1	D	100	PRO
1	D	106	THR
1	D	118	THR
1	D	119	ASP
1	D	142	LEU
1	D	159	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	19	ASN
1	A	30	GLN
1	A	155	GLN
1	B	19	ASN
1	B	30	GLN
1	B	155	GLN
1	C	19	ASN
1	C	30	GLN
1	C	155	GLN
1	D	19	ASN
1	D	30	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	51	ASN
1	D	155	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](#)

4 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
2	SCN	D	176	-	1,2,2	0.70	0	0,1,1	-	-
2	SCN	C	176	-	1,2,2	0.87	0	0,1,1	-	-
2	SCN	B	176	-	1,2,2	0.51	0	0,1,1	-	-
2	SCN	A	176	-	1,2,2	0.98	0	0,1,1	-	-

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.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	176	SCN	2	0
2	C	176	SCN	1	0
2	A	176	SCN	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled '#RSRZ > 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	156/175 (89%)	-1.30	0 100 100	12, 25, 53, 70	0
1	B	156/175 (89%)	-1.33	0 100 100	13, 24, 52, 68	0
1	C	156/175 (89%)	-1.33	0 100 100	12, 25, 51, 70	0
1	D	156/175 (89%)	-1.32	0 100 100	11, 25, 50, 68	0
All	All	624/700 (89%)	-1.32	0 100 100	11, 25, 52, 70	0

There are no RSRZ outliers to report.

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

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

### 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	SCN	B	176	3/3	0.98	0.05	23,23,25,48	0
2	SCN	A	176	3/3	0.99	0.04	9,9,16,45	0
2	SCN	C	176	3/3	0.99	0.04	8,8,9,46	0
2	SCN	D	176	3/3	0.99	0.05	18,18,24,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.