Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 11:00 PM GMT

PDB ID	:	5EZP
Title	:	Human transthyretin (TTR) complexed with 4-hydroxy-chalcone
Authors	:	Polsinelli, I.; Nencetti, S.; Shepard, W.E.; Orlandini, E.; Stura, E.A.
Deposited on	:	2015-11-26
Resolution	:	2.50 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see references ⓘ) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982
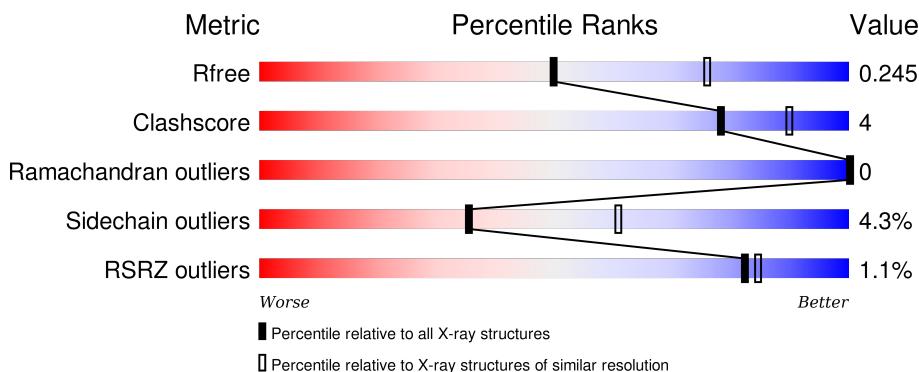
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	Percentile Ranks	Value
Rfree		0.245
Clashscore		4
Ramachandran outliers		0
Sidechain outliers		4.3%
RSRZ outliers		1.1%

Worse ← → *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	122	85% 9% 6%
1	B	122	88% 5% · ·
1	C	122	81% 11% · ·
1	D	122	2% 79% 7% 9% 5%
1	E	122	3% 85% 13% ·

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Mol	Chain	Length	Quality of chain
1	F	122	84% 11%
1	G	122	91% 6%
1	H	122	82% 10% 7%

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	IPJ	A	201	-	-	-	X
2	IPJ	B	201	-	-	-	X
2	IPJ	C	201	-	-	-	X
2	IPJ	F	201	-	-	-	X
2	IPJ	G	202	-	-	-	X

2 Entry composition (i)
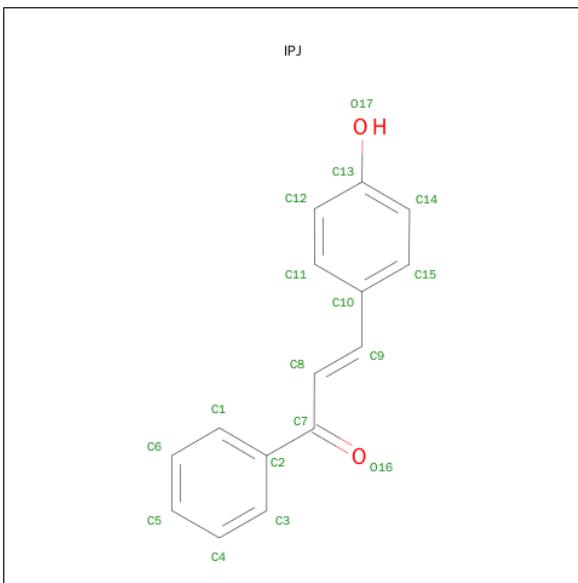
There are 4 unique types of molecules in this entry. The entry contains 7740 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Transthyretin.
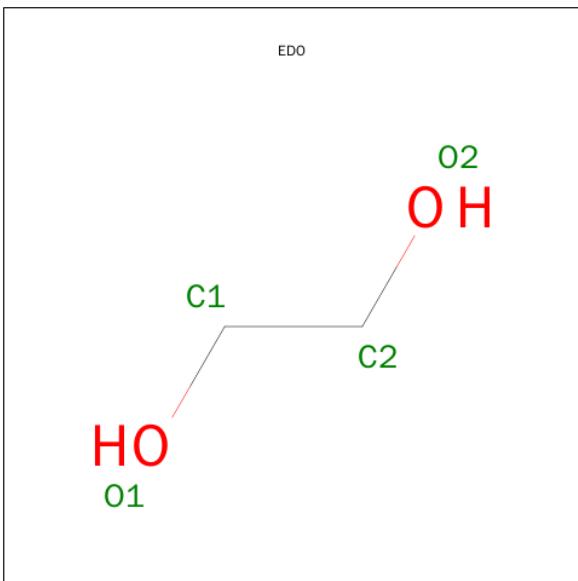
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	115	Total 899	C 575	N 147	O 176	S 1	0	1	0
1	B	117	Total 909	C 581	N 149	O 178	S 1	0	0	0
1	C	117	Total 918	C 586	N 150	O 181	S 1	0	1	0
1	D	116	Total 899	C 576	N 148	O 174	S 1	0	0	0
1	E	122	Total 943	C 600	N 155	O 186	S 2	0	0	0
1	F	117	Total 909	C 581	N 149	O 178	S 1	0	0	0
1	G	118	Total 953	C 605	N 157	O 189	S 2	0	4	0
1	H	114	Total 892	C 571	N 147	O 173	S 1	0	1	0

• Molecule 2 is 4-hydroxy-chalcone (three-letter code: IPJ) (formula: $C_{15}H_{12}O_2$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 17	C 15	O 2	0	0
2	B	1	Total 17	C 15	O 2	0	0
2	C	1	Total 17	C 15	O 2	0	0
2	F	1	Total 17	C 15	O 2	0	0
2	G	1	Total 17	C 15	O 2	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	1	Total 4	C 2	O 2	0	0
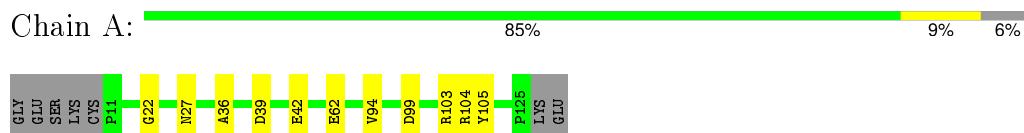
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	40	Total 40	O 40	0	0
4	B	41	Total 41	O 41	0	0
4	C	48	Total 48	O 48	0	0
4	D	37	Total 37	O 37	0	0
4	E	46	Total 46	O 46	0	0
4	F	43	Total 43	O 43	0	0
4	G	39	Total 39	O 39	0	0
4	H	35	Total 35	O 35	0	0
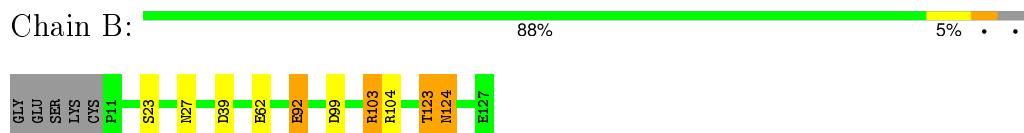
3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.
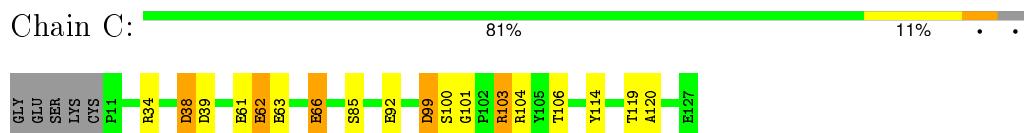
- Molecule 1: Transthyretin
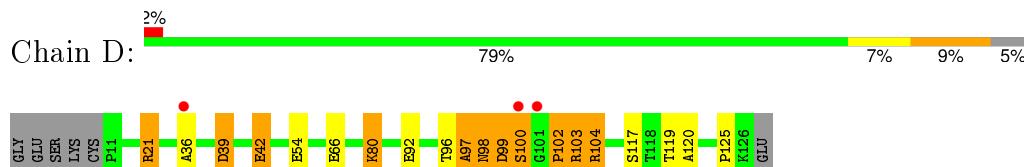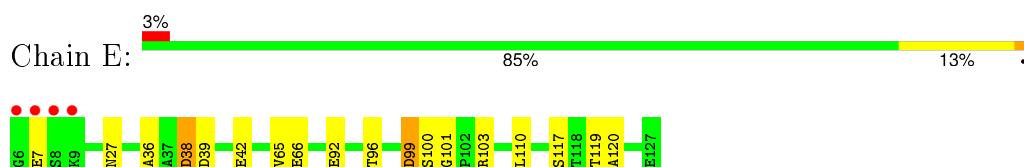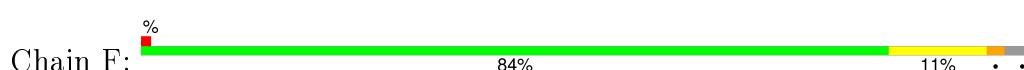
- Molecule 1: Transthyretin

- Molecule 1: Transthyretin

- Molecule 1: Transthyretin

- Molecule 1: Transthyretin

- Molecule 1: Transthyretin

GLY GLU SER LYS CYS | P11 | R34 | K35 | A36 | D39 | E42 | L58 | E61 | E72 | K76 | K80 | E92 | D99 | R103 | T119 | A120 | E127

- Molecule 1: Transthyretin

Chain G:

2%

91%   6%

GLY GLU SER LYS | C10 | D39 | E51 | E63 | E92 | D99 | S117 | K126 | E127

- Molecule 1: Transthyretin

Chain H:

82%   10%   7%

GLY GLU SER LYS CYS | P11 | L12 | M13 | K35 | A36 | A37 | D38 | D39 | T40 | W41 | E42 | E63 | K80 | E92 | D99 | R103 | S117 | T123 | N124 | PRO LYS GLU
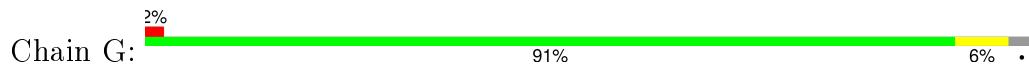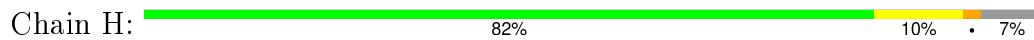
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	62.48Å 62.48Å 238.32Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.72 – 2.50 44.72 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.72-2.50) 99.6 (44.72-2.50)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	0.19	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.210 , 0.245 0.210 , 0.245	Depositor DCC
R_{free} test set	1783 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	45.5	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 31.7	EDS
Estimated twinning fraction	0.069 for -h,-k,l 0.257 for h,-h-k,-l 0.086 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Outliers	0 of 35643 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7740	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< \|L\| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: IPJ, EDO

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	0.95	0/923	0.94	3/1259 (0.2%)
1	B	0.93	0/933	0.98	3/1270 (0.2%)
1	C	0.97	1/942 (0.1%)	1.07	6/1282 (0.5%)
1	D	1.11	2/923 (0.2%)	1.21	14/1258 (1.1%)
1	E	0.87	0/967	0.97	4/1315 (0.3%)
1	F	1.00	2/933 (0.2%)	0.96	5/1270 (0.4%)
1	G	0.96	0/977	0.94	1/1329 (0.1%)
1	H	0.91	0/915	0.98	3/1246 (0.2%)
All	All	0.97	5/7513 (0.1%)	1.01	39/10229 (0.4%)

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	H	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	102	PRO	CA-C	6.38	1.65	1.52
1	D	42	GLU	CD-OE2	6.36	1.32	1.25
1	F	72	GLU	CD-OE2	6.01	1.32	1.25
1	C	66	GLU	CG-CD	5.99	1.60	1.51
1	F	61	GLU	CB-CG	5.31	1.62	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	38	ASP	CB-CG-OD1	10.90	128.11	118.30
1	C	34	ARG	NE-CZ-NH1	-10.25	115.17	120.30
1	D	39	ASP	CB-CG-OD1	9.81	127.13	118.30
1	E	38	ASP	N-CA-CB	-8.68	94.98	110.60
1	D	96	THR	CA-CB-CG2	-8.27	100.83	112.40
1	E	38	ASP	CB-CG-OD1	8.26	125.73	118.30
1	D	97	ALA	N-CA-C	-7.77	90.03	111.00
1	D	39	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	D	100	SER	N-CA-C	7.38	130.92	111.00
1	D	104	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	D	97	ALA	CB-CA-C	7.29	121.03	110.10
1	F	80	LYS	CB-CG-CD	7.12	130.12	111.60
1	C	99	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	D	80	LYS	CB-CG-CD	7.00	129.81	111.60
1	H	13	MET	CB-CA-C	6.83	124.06	110.40
1	C	103	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	G	99	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	F	99	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	A	104	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	B	104	ARG	CB-CA-C	6.44	123.28	110.40
1	D	98	ASN	CA-C-N	-6.31	103.31	117.20
1	F	103	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	99	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	B	103	ARG	CG-CD-NE	-6.09	99.02	111.80
1	D	103	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	C	66	GLU	OE1-CD-OE2	-6.04	116.05	123.30
1	H	103	ARG	CG-CD-NE	5.96	124.31	111.80
1	C	34	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	F	34	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	D	104	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	99	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	D	54	GLU	OE1-CD-OE2	-5.39	116.84	123.30
1	D	21	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	F	34	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	D	42	GLU	CA-CB-CG	-5.28	101.79	113.40
1	E	99	ASP	N-CA-CB	-5.12	101.38	110.60
1	H	99	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	E	99	ASP	CB-CG-OD2	-5.07	113.74	118.30
1	A	62	GLU	N-CA-CB	5.04	119.67	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	123	THR	Peptide

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	899	0	870	5	0
1	B	909	0	884	5	0
1	C	918	0	889	12	0
1	D	899	0	878	11	0
1	E	943	0	915	14	0
1	F	909	0	884	8	0
1	G	953	0	915	5	0
1	H	892	0	870	5	0
2	A	17	0	11	0	0
2	B	17	0	11	1	0
2	C	17	0	11	1	0
2	F	17	0	12	0	0
2	G	17	0	11	3	0
3	G	4	0	6	0	0
4	A	40	0	0	0	0
4	B	41	0	0	1	0
4	C	48	0	0	0	0
4	D	37	0	0	2	0
4	E	46	0	0	1	0
4	F	43	0	0	4	0
4	G	39	0	0	1	0
4	H	35	0	0	0	0
All	All	7740	0	7167	52	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 (52) 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:F:76:LYS:HE2	1:F:80:LYS:HE3	1.47	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:ALA:HB1	1:D:100:SER:HB3	1.53	0.90
1:A:94:VAL:HG23	1:B:92:GLU:OE2	1.81	0.80
1:C:101:GLY:CA	1:E:99:ASP:OD1	2.39	0.71
1:C:101:GLY:N	1:E:99:ASP:OD1	2.23	0.71
1:C:61:GLU:HG2	1:C:62:GLU:HG3	1.75	0.69
1:D:103:ARG:NH1	4:D:201:HOH:O	2.28	0.66
1:C:101:GLY:HA2	1:E:99:ASP:OD1	1.97	0.64
1:D:99:ASP:O	1:D:102:PRO:HD2	1.96	0.64
1:F:11:PRO:N	4:F:301:HOH:O	2.31	0.64
1:E:65:VAL:HG22	1:E:66:GLU:N	2.14	0.62
1:H:38:ASP:OD1	1:H:40:THR:HG22	1.99	0.62
1:D:97:ALA:CB	1:D:100:SER:HB3	2.30	0.59
1:D:80:LYS:HD3	4:F:322:HOH:O	2.03	0.59
1:E:110:LEU:HD22	2:G:202:IPJ:C6	2.33	0.58
1:C:92:GLU:OE1	1:D:92:GLU:OE1	2.24	0.55
1:A:94:VAL:CG2	1:B:92:GLU:OE2	2.54	0.54
1:B:103:ARG:NH1	4:B:301:HOH:O	2.39	0.54
1:D:36:ALA:HB2	1:D:42:GLU:HG3	1.90	0.54
1:G:92[B]:GLU:HG2	1:H:92:GLU:OE1	2.09	0.53
1:E:101:GLY:HA2	1:E:103:ARG:HG2	1.91	0.52
1:E:36:ALA:HB2	1:E:42:GLU:HG3	1.91	0.52
1:E:65:VAL:CG2	1:E:66:GLU:N	2.73	0.52
1:E:110:LEU:HD22	2:G:202:IPJ:H4	1.90	0.52
1:D:21:ARG:NH1	4:D:202:HOH:O	2.36	0.51
1:B:124:ASN:OD1	1:B:124:ASN:N	2.45	0.50
1:D:66:GLU:OE1	1:D:98:ASN:O	2.31	0.48
1:F:119:THR:HG22	1:F:120:ALA:N	2.29	0.47
1:B:123:THR:HG23	2:C:201:IPJ:C15	2.44	0.47
1:F:58:LEU:HA	4:F:326:HOH:O	2.15	0.47
1:G:92[B]:GLU:HG2	1:H:92:GLU:CD	2.34	0.47
1:E:92:GLU:OE1	1:F:92:GLU:OE1	2.33	0.46
1:C:66:GLU:OE2	1:F:80:LYS:NZ	2.40	0.46
1:F:103:ARG:NH1	4:F:303:HOH:O	2.49	0.46
1:A:22:GLY:HA3	1:C:114:TYR:CD2	2.51	0.46
1:G:92[B]:GLU:OE2	4:G:301:HOH:O	2.20	0.45
1:D:104:ARG:NH2	1:D:125:PRO:HB3	2.32	0.45
1:G:92[B]:GLU:CD	1:G:92[B]:GLU:H	2.20	0.44
2:G:202:IPJ:C3	2:G:202:IPJ:H7	2.48	0.44
1:C:103:ARG:NH2	1:E:66:GLU:OE1	2.50	0.44
2:B:201:IPJ:H7	1:C:106:THR:HG21	1.99	0.43
1:D:119:THR:HG22	1:D:120:ALA:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:119:THR:HG22	1:E:120:ALA:N	2.32	0.43
1:A:36:ALA:HB2	1:A:42:GLU:HG3	2.01	0.42
1:E:27:ASN:ND2	4:E:204:HOH:O	2.52	0.42
1:H:36:ALA:HB2	1:H:42:GLU:HG3	2.01	0.42
1:C:100:SER:HA	1:E:96:THR:HG21	2.00	0.42
1:F:36:ALA:HB2	1:F:42:GLU:HG3	2.03	0.41
1:A:103:ARG:HB2	1:A:105:TYR:CE1	2.55	0.41
1:C:99:ASP:OD1	1:C:99:ASP:C	2.59	0.41
1:C:119:THR:HG22	1:C:120:ALA:N	2.34	0.41
1:G:117:SER:HB2	1:H:117:SER:HB2	2.02	0.41

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	114/122 (93%)	112 (98%)	2 (2%)	0	100	100
1	B	115/122 (94%)	113 (98%)	2 (2%)	0	100	100
1	C	116/122 (95%)	114 (98%)	2 (2%)	0	100	100
1	D	114/122 (93%)	110 (96%)	4 (4%)	0	100	100
1	E	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
1	F	115/122 (94%)	109 (95%)	6 (5%)	0	100	100
1	G	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
1	H	113/122 (93%)	107 (95%)	6 (5%)	0	100	100
All	All	927/976 (95%)	900 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	97/102 (95%)	95 (98%)	2 (2%)	61	85
1	B	98/102 (96%)	91 (93%)	7 (7%)	18	34
1	C	99/102 (97%)	93 (94%)	6 (6%)	23	42
1	D	97/102 (95%)	94 (97%)	3 (3%)	47	75
1	E	102/102 (100%)	97 (95%)	5 (5%)	31	55
1	F	98/102 (96%)	97 (99%)	1 (1%)	82	95
1	G	103/102 (101%)	97 (94%)	6 (6%)	25	45
1	H	96/102 (94%)	90 (94%)	6 (6%)	22	40
All	All	790/816 (97%)	754 (95%)	36 (5%)	35	57

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ASN
1	A	39	ASP
1	B	23	SER
1	B	27	ASN
1	B	39	ASP
1	B	62	GLU
1	B	92	GLU
1	B	123	THR
1	B	124	ASN
1	C	38	ASP
1	C	39	ASP
1	C	62	GLU
1	C	63	GLU
1	C	85	SER
1	C	104	ARG
1	D	39	ASP
1	D	99	ASP
1	D	117	SER
1	E	7	GLU

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Mol	Chain	Res	Type
1	E	38	ASP
1	E	39	ASP
1	E	100	SER
1	E	117	SER
1	F	39	ASP
1	G	10	CYS
1	G	39	ASP
1	G	51[A]	GLU
1	G	51[B]	GLU
1	G	63[A]	GLU
1	G	63[B]	GLU
1	H	13	MET
1	H	35	LYS
1	H	39	ASP
1	H	63	GLU
1	H	80	LYS
1	H	92	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates 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	#$|Z| > 2$
2	IPJ	A	201	-	18,18,18	0.82	0	23,23,23	1.88	4 (17%)
2	IPJ	B	201	-	18,18,18	0.70	0	23,23,23	1.18	2 (8%)
2	IPJ	C	201	-	18,18,18	0.67	0	23,23,23	0.89	1 (4%)
2	IPJ	F	201	-	18,18,18	0.68	0	23,23,23	0.82	1 (4%)
3	EDO	G	201	-	3,3,3	0.52	0	2,2,2	0.28	0
2	IPJ	G	202	-	18,18,18	0.82	0	23,23,23	1.13	1 (4%)

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
2	IPJ	A	201	-	-	0/9/9/9	0/2/2/2
2	IPJ	B	201	-	-	0/9/9/9	0/2/2/2
2	IPJ	C	201	-	-	0/9/9/9	0/2/2/2
2	IPJ	F	201	-	-	0/9/9/9	0/2/2/2
3	EDO	G	201	-	-	0/1/1/1	0/0/0/0
2	IPJ	G	202	-	-	0/9/9/9	0/2/2/2

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	201	IPJ	C10-C9-C8	-2.67	120.81	126.98
2	A	201	IPJ	O16-C7-C8	-2.43	116.97	120.89
2	B	201	IPJ	O16-C7-C2	-2.04	115.55	119.07
2	F	201	IPJ	C1-C2-C3	2.11	121.50	118.61
2	C	201	IPJ	C2-C7-C8	2.41	122.10	119.23
2	G	202	IPJ	C9-C8-C7	2.77	126.05	121.49
2	B	201	IPJ	C2-C7-C8	4.47	124.54	119.23
2	A	201	IPJ	C9-C8-C7	4.92	129.62	121.49
2	A	201	IPJ	C2-C7-C8	6.03	126.40	119.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	201	IPJ	1	0
2	C	201	IPJ	1	0
2	G	202	IPJ	3	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	115/122 (94%)	-0.44	0	100	100	28, 44, 68, 95	0
1	B	117/122 (95%)	-0.31	0	100	100	33, 50, 85, 107	0
1	C	117/122 (95%)	-0.42	0	100	100	29, 43, 78, 112	0
1	D	116/122 (95%)	-0.22	3 (2%)	59	63	29, 47, 94, 125	0
1	E	122/122 (100%)	-0.19	4 (3%)	50	55	27, 49, 101, 140	0
1	F	117/122 (95%)	-0.46	1 (0%)	85	88	29, 41, 68, 117	0
1	G	118/122 (96%)	-0.34	2 (1%)	73	76	29, 44, 79, 114	0
1	H	114/122 (93%)	-0.39	0	100	100	30, 47, 79, 95	0
All	All	936/976 (95%)	-0.35	10 (1%)	82	84	27, 45, 84, 140	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	6	GLY	4.8
1	D	100	SER	3.9
1	G	126	LYS	3.7
1	E	8	SER	3.4
1	D	101	GLY	2.4
1	E	7	GLU	2.3
1	G	127	GLU	2.3
1	E	9	LYS	2.2
1	F	127	GLU	2.0
1	D	36	ALA	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	IPJ	A	201	17/17	0.82	0.39	12.01	74,77,83,100	0
2	IPJ	G	202	17/17	0.84	0.33	10.53	73,79,82,88	0
2	IPJ	C	201	17/17	0.60	0.68	8.36	110,117,123,123	0
2	IPJ	B	201	17/17	0.87	0.35	7.94	81,85,103,115	0
2	IPJ	F	201	17/17	0.91	0.26	5.12	71,80,96,98	0
3	EDO	G	201	4/4	0.88	0.12	-	63,67,68,70	0

6.5 Other polymers (i)

There are no such residues in this entry.